THE THEORY OF S-FUNCTIONS

AND APPLICATIONS IN QUANTUM MECHANICS

A thesis presented for the degree of
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by

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To My Wife

To My Parents.

A B S T R A C T

S-functions, as developed by D.E. Littlewood, are reviewed and their properties developed and extended. A computer programme has been written to perform most S-function operations. In particular, S-function division is defined, which produces many simplifications, and general methods for calculating both inner and outer plethysm are derived.

The properties of matrix groups are similarly discussed using the theory of S-functions and programmes written to produce branching rules and Kronecker products. This required some new work on spin characters and on the difference characters of even dimensional rotation groups.

Generalized Racah tensors are used to study the group properties of general mixed configurations of electrons. Some properties of factorized general coupling and recoupling coefficients are also derived. These properties are used to calculate part of general two body fractional parentage coefficients.

The above methods are used to investigate the usefulness of the group R_4 as an approximate symmetry for the first row atoms. It is found that the interaction with the underlying $1s^2$ shell completely breaks this symmetry.

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INTRODUCTION

In the past decade theoretical physicists have shown great interest in the theory of continuous groups for application to a wide range of physical problems. Notable, among the many uses, has been that of the compact continuous groups, to describe the transformation properties of N-particle atomic and nuclear wave-functions. This use was pioneered by Racah[1,2] and physicists have tended to concentrate on an approach, in the tradition of Elie Cartan[3] and Sophus Lie[4], of considering the properties of infinitesimal transformations. Hermann Weyl's book, "The Classical Groups"[5], has undoubtably exercised a considerable influence on these developments.

For much of this thesis I intend to use an alternative approach to the theory of continuous groups. This approach complements the earlier work of Cartan and Lie, and has been developed by D.E. Littlewood as a consequence of Schur's original thesis[6] on the properties of invariant matrices. Littlewood's treatment[7,8] circumvents the study of infinitesimal transformations by considering the properties of special functions of the roots of the matrices that characterize the elements of the continuous groups. This approach obviates constructing the group characters explicitly. These functions, known as Schur functions, or simply S-functions, have been used by Littlewood to find relatively simple formulae connecting the characters of representation of the unitary symplectic, orthogonal and rotation groups.

The first half of this thesis is concerned with a systemization of Littlewood's methods, with the aim of writing computer programmes that perform all required operations with characters of the symmetric and the continuous groups. Unlike other authors, I prefer to introduce S-functions as simple algebraic entities, which we may combine together in several ways. From the well-known[9,10] outer multiplication of S-functions, I am led to a concept of division of S-functions. This new operation not only considerably simplifies calculations, but leads to a new insight into many of the relations (e.g. the canonical chain for rotation groups).

Using these two operations and a theorem by Littlewood it is a simple matter to write a programme for the systematic evaluation of inner products of S-functions, without the use of character tables. The operations of inner and outer plethysm have presented even more difficulties in the past. A little known recursion relation due to Murnaghan provides the key to the machine calculation of outer plethysm. I prefer to regard this operation as a substitution[11] or as a symmetrized product[10] rather than as an immanant of an immanant[8]. In order to calculate inner plethysms I develop the algebra to the stage where it will be a simple matter to write a programme remarkably similar to the outer plethysm programme.

Chapter two briefly outlines some of the properties of the generating functions that may be used to prove the results of Chapter one. Using these methods two new special series required in the following chapter are derived. The S-functions generated by such special series are basic to the treatment in Chapter three of the matrix representation theory of the continuous groups.

The beginning of this next chapter is a brief outline of how to obtain integration formulae and class functions for the continuous groups. Littlewood uses the theory of immanants to obtain the group characters, but since this requires much knowledge of matrix theory, I use an approach more akin to that of Murnaghan[12-14], although, of course, the use of S-functions is based on Littlewood's text[7]. In the course of deriving the spin characters of the rotation groups, I have noted several corrections to Littlewood's text (appendix I). The large part of this chapter is, however, concerned with systematizing the algebra of representation theory. Results due to Littlewood, Judd and others, are used to give a direct means of machine calculation of Kronecker products and of branching rules. This required that I resolve the various products of the basic spin and difference characters of the rotation groups. The resolution of the Kronecker squares of these characters is also derived including the dimension check, since these are required for selection rules. I finish the chapter by re-deriving the canonical chain for all characters of rotation groups, to show how trivial an otherwise complicated problem becomes when using the algebra of S-functions.

Almost all of the algebra of S-functions and of character theory discussed here has been programmed. The important exception is the inner plethysm, but the method derived here is now directly amenable. The seventh chapter discusses some of the computing problems. A large number (200 pages) of tables are being published[32] and Appendix III gives only representative output of programmes written since then.

The other three chapters are more in the approach commonly used by physicists. Chapter four generalizes work done by Feneuille and others on mixed configurations, using the methods of Racah tensors, but in choosing subgroups we bear in mind the fact that R_4 is an exact symmetry for the bound states of the non-relativistic hydrogen atom. I study various choices for the linear combinations of $\underset{\sim}{v}^{(k)}(\ell_a,\ell_b)$ and $\underset{\sim}{v}^{(k)}(\ell_b,\ell_a)$ required to form these subgroups. After defining a suitable combination, I obtain the commutation relations and hence construct all non-exceptional root figures. The transformation properties of states and operators under the rotation and symplectic groups follow easily, but I also derive the transformation properties of the operators under unitary operations. General Casimir operators and eigenvalues are given in terms of these Racah tensors. A general expression for the inter-electronic coulomb interaction is also given.

Much work is being done at the present on the calculation of generalized coupling coefficients. Various papers have been published on the symmetry properties of the coupling coefficients

$$\langle w_1 m_1 ; w_2 m_2 | \gamma\, wm \rangle$$

where the ket $|wm\rangle$ is the m^{th} ket spanning the representation w, γ being an additional label required if w appears more than once in the Kronecker product $w_1 \times w_2$. However, physicists are usually interested in a group chain and write a ket as $|WULM\rangle$ (multiplicity labels suppressed). The resultant coupling coefficients may be factored by the Wigner-Eckart theorem. In Chapter five I derive several new results concerning these coefficients, and am thus able to obtain, quite generally, the square of the two-body coefficients of fractional parentage for the part of the chain

$$U_{2x} \rightarrow Sp_{2x} \rightarrow SU_2 \times R_x.$$

In Chapter six all these various ideas are used to decide how much the R_4 symmetry is broken by inter-electronic coulombic forces in a non-hydrogenic atom. The interaction is symmetrized under R_4 operations and the effect of various radial functions observed. With either hydrogenic or Hartree Fock wave-functions it is found that, contrary to previous results, the R_4 symmetry is completely broken. The symmetry is primarily broken by the underlying closed shells of electrons.

CHAPTER I

S-FUNCTIONAL ANALYSIS

The S-function may be defined without reference to group theory, and few basic tools of combinatorial analysis are required. In the main this approach is that of Littlewood[7] and most results may be proved using generating functions (see Chapter II), but we shall not attempt a rigorous development here.

Our approach has the advantage that theorems do not require use of group properties for their proof, and more importantly, we do not require the use of symmetric group characters, which would otherwise be essential. While these characters have been evaluated for symmetric groups up to S_{16}, they are very difficult to use except in simple cases.

1. FUNDAMENTAL NOTIONS

Partitions: A set of r positive integers whose sum is n is said to form a partition of n. An ordered partition is one where the integers are ordered from largest to smallest (or vice versa). All partitions henceforth, will be so ordered with the notation that a Greek letter will denote a general partition so: (λ) or $(\lambda_1,\lambda_2,\cdots\lambda_r)$, and this will be assumed to be a partition of n. A Latin letter will denote a partition into one part only. A Young diagram is associated with each partition. It is the graph of r rows, λ_i dots (or squares) in the i^{th} row, with each row left justified. A conjugate partition is formed by interchanging the rows and columns of the graph, and will be denoted by $(\tilde{\lambda})$

$$\text{e.g.}\quad (322) \sim \begin{matrix} o & o & o \\ o & o & \\ o & o & \end{matrix} \qquad\qquad (331) \sim \begin{matrix} o & o & o \\ o & o & o \\ o & & \end{matrix}$$

We see that $(\widetilde{322}) = (331)$.

Some partitions are self-conjugates, e.g. (332). Partitions with repeated parts are often written with a superscript denoting the number of times the part occurs, thus $(33221) = (3^2 2^2 1)$.

Frobenius' notation is sometimes of use. The leading diagonal of the Young diagram is defined to be the one that starts in the top left hand corner. For each dot on the diagonal we write down the number of dots to the right of it, and below this, the number of dots beneath it. Thus

$$(5^2 41^2) = \begin{pmatrix} 4 & 3 & 1 \\ 4 & 1 & 0 \end{pmatrix} \quad \text{and} \quad (2^2) = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}.$$

```
o  o  o  o  o  4          o  o  1
o  o  o  o  o  3          o  o  0
o  o  o  o     1          1  0
o
o
4  1  0
```

N.B. The zeros are significant.

Young Tableaux: The term Young tableau is used to refer to a Young diagram which has its cells labelled in some fashion.

If we label a diagram corresponding to a partition of n by the numbers 1, 2,$\cdots$, n without restricting the ways, there will be n! possible tableaux.

Symmetric Functions: A symmetric function on k variables α_i is one that is unchanged by any permutation of the variables. Two such functions are of interest in this chapter.

1) Mononomial Symmetric functions - if (ρ) is a partition we define the mononomial S_ρ such that

$$M_\rho = \Sigma\alpha_1^{\rho_1}\alpha_2^{\rho_2}\cdots\alpha_r^{\rho_r}. \qquad (1.1)$$

where the summation is over all different permutations of the α's. For example, if k = 3, $M_{(11)} = \alpha_1\alpha_2 + \alpha_2\alpha_3 + \alpha_3\alpha_1$.

2) Homogeneous Product Sums, h_n - The homogeneous product sum h_n is defined to be the sum over all of the mononomials M_ρ, ρ being a partition of n.

$$h_n = \sum_\rho M\rho . \tag{1.2}$$

2. S-FUNCTIONS

If (λ) is a partition of n, the S-function $\{\lambda\}$ is the determinant of the h_i's defined as follows:

$$\{\lambda\} = |h_{\lambda_s - s+t}| \tag{1.3}$$

the s and t being subscripts for the row and column respectively. We extend the definition of the homogeneous product sums to include $h_0 = 1$ and $h_i = 0$ if $i < 0$.

Thus

$$\{311\} = \begin{vmatrix} h_3 & h_4 & h_5 \\ h_0 & h_1 & h_2 \\ 0 & h_0 & h_1 \end{vmatrix} = h_3h_1h_1 - h_3h_2 - h_4h_1 + h_5$$

also $\{n\} = |h_n| = h_n$.

The Symmetric Group: Under the operations of the group the symmetric group S_n with n! elements is split into classes ρ with h_ρ elements. Each class is the complete set of conjugates of a given element. The irreducible representations of the group may be placed into a one to one correspondence with the partitions on n. Because conjugate matrices have the same characteristic (i.e. spur or trace) there exists a unique number $\chi_\rho^{(\lambda)}$; the characteristic for a particular class of a representation. The set of characteristics of a representation is known as the character of the representation. If we define a function

$$\{\lambda\} = \sum_\rho \frac{h_\rho}{n!} \chi_\rho^{(\lambda)} M_\rho \tag{1.4}$$

we may prove that it is in complete correspondence with the representations of the symmetric group.

Littlewood[7] has shown that this definition is entirely equivalent to the definition of the S-function given earlier, to give us a complete isomorphism between operations on S-functions and operations on representations of the symmetric groups.

<u>The Degree of an S-function:</u> The degree (or dimension) of a representation of the symmetric group has been derived a number of ways by different workers. Because of the close correspondence between S_n and the S-functions corresponding to a partition of n we often talk of the degree of the S-function.

The degree of the representation $\{\lambda\}$ is

$$f\{\lambda\} = \frac{n! \prod_{i<j=1}^{r} (\lambda_i - \lambda_j + j - i)}{\prod_{i=1}^{r} (\lambda_i + r - i)!} \qquad (1.5)$$

where $\{\lambda\}$ is a partition of n into r parts. A formula more suited to hand calculation, given in terms of a concept of "hook lengths", is derived by Robinson[10].

3. EXPANSION OF AN S-FUNCTION IN TERMS OF THE VARIABLES

It is of interest to reverse the procedure for defining an S-function and to be able to write down the expression of the S-function in terms of the basic variables. Littlewood gives us a graphical method of doing this:

Firstly we draw the graph of the partition λ and then we label the cells in all possible ways such that

1) reading across the graph the labels are non-decreasing,

2) reading down the graph the labels are strictly increasing,

3) when we write down how many labels we have of each kind, then we must have an ordered partition.

The list of partitions are the mononomials that form the S-function. We may produce the sum of variables by taking the appropriate powers and products for all permutations of the variables suffices.

For example, to obtain the expansion of {31} we obtain

$$\begin{array}{lll} \alpha & \alpha & \alpha \\ \beta & & \end{array} \qquad \begin{array}{lll} \alpha & \alpha & \beta \\ \beta & & \end{array} \qquad \begin{array}{lll} \alpha & \alpha & \beta \\ \gamma & & \end{array} \qquad \begin{array}{lll} \alpha & \alpha & \gamma \\ \beta & & \end{array} \qquad \begin{array}{lll} \alpha & \beta & \gamma \\ \delta & & \end{array}$$

$$\begin{array}{lll} \alpha & \beta & \delta \\ \gamma & & \end{array} \qquad \begin{array}{lll} \alpha & \gamma & \delta \\ \beta & & \end{array}$$

giving {31} = (31) + (22) + 2(211) + 3(1111).

If the S-function is on the three variables $x_1\ x_2\ x_3$ the mononomials (1111) are null and the others give rise to the terms

$$x_1{}^3x_2 + x_1{}^3x_3 + x_2{}^3x_1 + x_2{}^3x_3 + x_3{}^3x_1 + x_3{}^3x_2 + x_1{}^2x_2{}^2$$

$$+ x_1{}^2x_3{}^2 + x_2{}^2x_3{}^2 + 2(x_1{}^2x_2x_3 + x_1x_2{}^2x_3 + x_1x_2x_3{}^2)$$

4. OUTER MULTIPLICATION S-FUNCTIONS

An S-function $\{\lambda\}$, (λ) a partition on m, is a function of degree m on the variables $x_1,\cdots,x_m$, with particular symmetry properties. We may multiply together two such functions $\{\lambda\}$ and $\{\mu\}$, being functions of degree m and n respectively, to produce a function of degree m+n. This function will be, in general, reducible to a sum of functions

$\{\nu\}$ with the appropriate S-functional symmetries. The resolution of such a product - corresponding to a product of the representations $\{\lambda\}$ and $\{\mu\}$ of symmetric groups S_m and S_n to form representations $\{\nu\}$ of S_{m+n} - is known as the outer or ordinary multiplication of S-functions. It is of key importance in the algebra. The rules for performing the operation using the Young diagram representation have been given many times[7,9] although, so far as it is known, it has not suggested how to systematically cover all possibilities for the graphs.

The S-functions appearing in the product $\{\lambda\}\{\mu\} = \dot{\Sigma}\{\nu\}$ are those which can be built by adding to the graph of $\{\lambda\}$ μ_1 symbols α, μ_2 symbols β, μ_3 symbols γ, etc., in this order and in the ways specified by the following:

1) No two identical symbols appear in the same column of the graph.

2) If we count the α's, β's, γ's etc. from right to left, starting at the top, then at all times while the count is being made, the number of α's must be not less than the number of β's which must not be less than the number of γ's and so on.

3) The graphs we obtain after the addition of each symbol must be regular, i.e. the corresponding partition must be ordered.

The Principal Part of the product is the term obtained when the partitions are simply added, i.e. the partition $\{\lambda_1+\mu_1, \lambda_2+\mu_2, \cdots, \lambda_i+\mu_i, \cdots\}$. It corresponds graphically to putting all the α's in the first row, the β's in the second and so on. The other terms in the product may be systematically produced by removing the last element and trying it on the next lower line, then the next etc. When it will fit nowhere else remove the second to last element also. Try to fit this in the same fashion, if no place is found remove the third to last element, when one is found to fit try to replace the elements in their highest positions. Note also that, for example, for the third γ we may place it on the same line, or below, the second γ but not above it.

This operation is checked dimensionally by use of the equation

$$f\{\lambda\}f\{\mu\}\frac{(n+m)!}{n!m!} = \Sigma f\{\nu\}, \tag{1.5}$$

where (λ) is a partition of n, and (μ) of m. For example $\{31\}\{21\}$

$$\begin{array}{lll} o & o & o \\ o & & \end{array} \;\times\; \begin{array}{ll} o & o \\ o & \end{array} \;=\; \begin{array}{lllll} o & o & o & \alpha & \alpha \\ o & \beta & & & \end{array} \;+\; \begin{array}{lllll} o & o & o & \alpha & \alpha \\ o & & & & \\ \beta & & & & \end{array}$$

$$+ \begin{array}{llll} o & o & o & \alpha \\ o & \alpha & \beta & \end{array} + \begin{array}{llll} o & o & o & \alpha \\ o & \alpha & & \\ \beta & & & \end{array} + \begin{array}{llll} o & o & o & \alpha \\ o & \beta & & \\ \alpha & & & \end{array} + \begin{array}{llll} o & o & o & \alpha \\ o & & & \\ \alpha & & & \\ \beta & & & \end{array}$$

$$+ \begin{array}{lll} o & o & o \\ o & \alpha & \alpha \\ \beta & & \end{array} + \begin{array}{lll} o & o & o \\ o & \alpha & \\ \alpha & \beta & \end{array} + \begin{array}{lll} o & o & o \\ o & \alpha & \\ \alpha & & \\ \beta & & \end{array}$$

note that the graphs

$$\begin{array}{lll} o & o & o \\ o & \alpha & \beta \\ \alpha & & \end{array} \qquad \begin{array}{lll} o & o & o \\ o & & \\ \alpha & & \\ \alpha & & \\ \beta & & \end{array} \qquad \begin{array}{llll} o & o & o & \\ o & \alpha & \alpha & \beta \end{array} \qquad \begin{array}{lll} o & o & o \\ o & \beta & \alpha \\ \alpha & & \end{array}$$

all break the rules given above. Thus we obtain the expansion

$$\{31\}\{21\} = \{52\} + \{51^2\} + \{43\} + 2\{421\} + \{41^3\} + \{3^21\} + \{32^2\} + \{321^2\},$$

dimensionally

$$3.2\frac{7!}{4!3!} = 14 + 15 + 14 + 2.35 + 20 + 21 + 21 + 35.$$

5. S-FUNCTION DIVISION

Frequently the algebra requires the evaluation of the sum of S-functions $\{\nu\}$ which when multiplied by a particular S-function $\{\mu\}$ give a particular S-function $\{\lambda\}$, the coefficient of $\{\nu\}$ being the coefficient of $\{\lambda\}$ in the outer product. Hence I define the (outer) division of S-functions $\{\lambda\}/\{\mu\}$ to be:

$$\{\lambda\}/\{\mu\} = \sum_{\nu}\Gamma_{\mu\nu\lambda}\{\nu\} \tag{1.6}$$

where $\Gamma_{\mu\nu\lambda}$ is the same as the coefficient in the outer product

$$\{\mu\}\{\nu\} = \sum_{\lambda}\Gamma_{\mu\nu\lambda}\{\lambda\}. \tag{1.7}$$

The evaluation of the division is somewhat easier than each product, thus considerably simplifying the calculation.

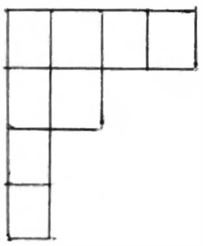
We have the graph of $\{\mu\}$ and wish to know all possible ways of adding elements to form the graph of $\{\lambda\}$ given the rules for the product. To evaluate the division, draw the graph for $\{\lambda\}$ with squares instead of dots, and fill up the left hand top corner with the graph corresponding to $\{\mu\}$. Graph $\{\mu\}$ must fit entirely inside $\{\lambda\}$ or the result must be null. The remaining squares are then labelled by

α's, β's, γ's etc. by rows, starting in the top left, as given by rules 1 and 2 of the product and also with:

3) The symbols must not decrease when reading left to right across a row, i.e. there must not be an α to the right of a β etc.

4) The resultant S-function must be ordered.

For example {4211}/{211}



$$/ \begin{array}{ll} o & o \\ o & \\ o & \end{array} = \begin{array}{llll} o & o & \alpha & \alpha \\ o & \alpha & & \\ o & & & \\ \alpha & & & \end{array} + \begin{array}{llll} o & o & \alpha & \alpha \\ o & \alpha & & \\ o & & & \\ \beta & & & \end{array}$$

$$+ \begin{array}{llll} o & o & \alpha & \alpha \\ o & \beta & & \\ o & & & \\ \alpha & & & \end{array} + \begin{array}{llll} o & o & \alpha & \alpha \\ o & \beta & & \\ o & & & \\ \beta & & & \end{array} + \begin{array}{llll} o & o & \alpha & \alpha \\ o & \beta & & \\ o & & & \\ \gamma & & & \end{array}$$

note that the graphs

$$\begin{array}{llll} o & o & \alpha & \beta \\ o & \alpha & & \\ o & & & \\ \alpha & & & \end{array} , \begin{array}{llll} o & o & \alpha & \alpha \\ o & \gamma & & \\ o & & & \\ \beta & & & \end{array}$$

are not allowed by the rules.

Thus

$$\{4211\}/\{211\} = \{4\} + 2\{31\} + \{22\} + \{211\}.$$

S-function division may also be performed by use of the properties of isobaric determinantal forms[7]

$$\{\lambda\}/\{\mu\} = |h_{\lambda_s-\mu_t-s+t}|$$

where λ_s is the s-th part of the partition (λ) and μ_t is the t-th part of the partition (μ) and thus s labels the rows and t the columns of the determinant. In the case of the preceding example we have

$$\{4211\}/\{211\} = \begin{vmatrix} h_2 & h_4 & h_5 & h_7 \\ 0 & h_1 & h_2 & h_5 \\ 0 & 0 & 1 & h_2 \\ 0 & 0 & 0 & h_1 \end{vmatrix}$$

$$= h_2h_1^2 = \{2\}\{1\}^2$$

$$= \{4\} + 2\{31\} + \{22\} + \{211\}$$

as before. In practice the preceding method is to be preferred for machine calculation. The notation $\{\lambda\}/\{\mu\}$ is to be preferred over $\{\lambda/\mu\}$ since we may easily show:

$$(\{\lambda\} + \{\mu\})/\{\nu\} = \{\lambda\}/\{\nu\} + \{\mu\}/\{\nu\} \tag{1.9}$$

$$(\{\lambda\}/\{\mu\})/\{\nu\} = (\{\lambda\}/\{\nu\})/\{\mu\} = \{\lambda\}/\{\mu\}/\{\nu\} \tag{1.10}$$

$$\{\lambda\}/(\{\mu\} + \{\nu\}) = \{\lambda\}/\{\mu\} + \{\lambda\}/\{\nu\} \qquad (1.11)$$

$$\{\lambda\}/\{\mu\}/\{\nu\} = \{\lambda\}/(\{\mu\}\{\nu\}) \qquad (1.12)$$

6. EXPRESSION OF AN S-FUNCTION IN SYMMETRIC PARTS

When an S-function is defined from character theory the problem of expressing it in terms of sums and differences of symmetric functions is a little difficult. However, the equivalence between that definition and our definition renders the problem trivial since our defining determinant is in terms of the h_r's.

$$\{\lambda\} = |h_{\lambda_s - s + t}|, \quad h_r = \{r\}. \qquad (1.13)$$

Sometimes it is useful to know the expansion of $\{\lambda\}$ in terms of products of the antisymmetric representations $\{1^r\}$. Because $h_r = \{\widetilde{1^r}\}$ we may take conjugates of the above relation. Alternatively we define the elementary symmetric function a_r as the mononomial corresponding to the partition (1^r)

$$a_r = {}^{M}(1^r) \qquad (1.14)$$

leading to the result[9]

$$\{\lambda\} = |a_{\tilde{\lambda}_s - s + t}|. \qquad (1.15)$$

In practice however, such a determinant is difficult to write down except in simple cases, owing to the very large number of terms (r!). The majority of these terms is zero and many others cancel. Instead one can systematically write

$$\{\lambda_1\lambda_2\cdots\lambda_r\} = \{\lambda_1\}\{\lambda_2\lambda_3\cdots\lambda_r\} \text{ - terms of more}$$

nearly symmetric representations.

7. INNER MULTIPLICATION OF S-FUNCTIONS

The inner multiplication of S-functions is defined as the product of two S-functions on the different variables $(x_1\cdots x_k)$, $(y_1\cdots y_\ell)$. It corresponds to a product of two representations of the same symmetric group. Its evaluation is considerably more complex than the outer product and cannot be done directly by a diagrammatic method. The S-functions $\{\lambda\}$ and $\{\mu\}$ must be of the same degree n in the variables (x_i), (y_j) and the product functions will be of degree n in the variables $(x_1,\cdots,x_k,y_1,\cdots y_\ell)$. Numerous attempts have been made to simplify the problem of resolving the product, with varying degrees of success. Most of these attempts have used the character table for the corresponding symmetric group, however, Littlewood[15] has developed a much more flexible method where the character tables are not required. The key theorem is

$$(\{\lambda\}\{\mu\})o\{\nu\} = \sum_{\rho,\sigma} \Gamma_{\rho\sigma\nu} (\{\lambda\}o\{\rho\})(\{\mu\}o\{\sigma\}) \tag{1.16}$$

where $\Gamma_{\rho\sigma\nu}$ has the usual meaning for the outer product. The symmtric representation is the identity element for this operation:

$$\{\lambda\}o\{n\} = \{\lambda\}, \tag{1.17}$$

(λ) a partition on n. Inner multiplication is distributive with respect to addition, hence all that is required for the evaluation of any inner product is for one S-function to be expressed in terms of symmetric parts, and the appropriate outer multiplications performed. To evaluate

$$\{\lambda\}o\{\mu\} = \Sigma g_{\lambda\mu\nu}\{\nu\} \tag{1.18}$$

the steps are

$$\{\lambda\} = \Sigma \{a\}\{b\} \cdots \{c\} \tag{1.19}$$

$$(\{a\}\{b\}\cdots\{c\})o\{\mu\} = \Sigma \Gamma_{\nu_a\nu_b \cdots \nu_c\mu} (\{\nu_a\}\{\nu_b\}\cdots\{\nu_c\}) \tag{1.20}$$

where (ν_i) is a partition of i, the sum is over all such partitions and $\Gamma_{\nu_a\nu_b\cdots\nu_c\mu}$ is the coefficient of μ in the outer product $\{\nu_a\}\{\nu_b\}\cdots\{\nu_c\}$.

We may check our result by noting:

$$f\{\lambda\}f\{\mu\} = \Sigma\, g_{\lambda\mu\nu}\, f\{\nu\}$$

Various relations among the coefficients are of importance

$$g_{\lambda\mu\nu} = g_{\tilde{\lambda}\tilde{\mu}\nu} \tag{1.21a}$$

$$g_{\lambda\mu\nu} = g_{\mu\lambda\nu} = g_{\lambda\nu\mu} \tag{1.21b}$$

The conjugate relations are of importance in listing tables of inner products, reducing the number by a factor of four. Relations (1.21b) express not only that the relation is Abelian, but that if we were to define inner division analogous to outer division, we would merely have the operation of inner multiplication:

$$\text{i.e. } \{\lambda\} \div \{\mu\} = \{\lambda\} \circ \{\mu\} \tag{1.22}$$

Trivial consequences of this are that the identity $\{n\}$ is contained only in products of the type $\{\lambda\}\circ\{\lambda\}$ and the antisymmetric representation $\{1^n\}$ is contained only in those of the type $\{\lambda\}\circ\{\tilde{\lambda}\}$.

8. THE OUTER PLETHYSM OF S-FUNCTIONS

An S-function $\{\lambda\}$, (λ) a partition of m is a function of degree m in the variables $x_1 \cdots x_k$. If we take the independent terms in the function (of the form $x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_k^{\alpha_k}$) as basic variables and substitute them in as the variables for an S-function $\{\mu\}$, degree n, we will have a function of degree mn in the original variables. Littlewood[16,17] has shown that this function can be resolved into a sum of S-functions $\{\nu\}$.

We write this operation of (outer) plethysm as

$$\{\lambda\} \otimes \{\mu\} \quad = \quad \Sigma G_{\lambda\mu\nu}\{\nu\} \tag{1.23}$$

If we take an n-fold product of $\{\lambda\}$ with itself then we will also get a sum of S-functions $\{\nu\}'$ of degree mn. The plethysm $\{\lambda\} \otimes \{\mu\}$ can be regarded as separating the n-fold product into a sum of "symmetrized outer products". We have in fact:

$$\{\lambda\}.\{\lambda\}\cdots n\text{ times} \quad = \quad \sum_{(\nu)} (f\{\nu\}).\{\lambda\} \otimes \{\nu\} \tag{1.24}$$

The coefficient in the expansion can be shown[10], using Schur's lemma, to be the dimension of the representation $\{\mu\}$ of S_n. The operation may be checked dimensionally by use of the equation

$$f(\{\lambda\}\otimes\{\mu\}) \quad = \quad \left(\frac{f\{\lambda\}}{m!}\right)^n \frac{f\{\mu\}}{n!}\,(mn)! \tag{1.26}$$

From its definition it follows that the operation is distributive on the right for addition and multiplication

$$\{\lambda\} \otimes (A\pm B) \quad = \quad \{\lambda\} \otimes A \pm \{\lambda\} \otimes B \tag{1.27}$$

$$\{\lambda\} \otimes (A.B) \quad = \quad (\{\lambda\} \otimes A)(\{\lambda\} \otimes B) \tag{1.28}$$

Plethysm may be carried out in any order

$$(\{\lambda\} \otimes \{\mu\}) \otimes \{\nu\} \quad = \quad \{\lambda\} \otimes (\{\mu\} \otimes \{\nu\}) \tag{1.29}$$

For operations on the left, cross terms appear in the substitution and we obtain the rules

$$(A+B) \otimes \{\lambda\} \quad = \quad \Sigma(A\otimes\{\mu\})(B\otimes(\{\lambda\}/\{\mu\})) \qquad (1.30)$$

$$(A-B) \otimes \{\lambda\} \quad = \quad \Sigma(A\otimes\{\lambda\}/\{\mu\}).(-)^{p}.(B\otimes\{\tilde{\mu}\}) \qquad (1.31)$$

$$(A.B) \otimes \{\lambda\} \quad = \quad \Sigma(A\otimes\{\mu\}).(B\otimes(\{\lambda\}\circ\{\mu\})) \qquad (1.32)$$

where the sums are over (μ) a partition of p. The inner product in eqn (1.32) restricts the sum to the partitions with $p = n$. A conjugate relation is useful:

$$\widetilde{\{\lambda\} \otimes \{\mu\}} \quad = \quad \{\tilde{\lambda}\} \otimes \{\mu\} \qquad n \text{ even} \qquad (1.33a)$$

$$= \quad \{\tilde{\lambda}\} \otimes \{\tilde{\mu}\} \qquad n \text{ odd} \qquad (1.33b)$$

(μ) a partition of n.

The theory of plethysm was approached by Littlewood from the theory of induced matrices and of immanants of matrices. A review of this approach may be found in P.R. Smith's thesis[18]. The approach given above is more akin to combinatorial analysis.

Much work in the 1950's went into finding a systematic method of calculating plethysms. Ibrahim[19] calculated tables of plethysms for $mn \leq 18$, by the use of the theorem:

$$(\{\lambda\}\otimes\{\mu\})/\{1\} \quad = \quad [\{\lambda\} \otimes (\{\mu\}/\{1\})][\{\lambda\}/\{1\}] \qquad (1.34)$$

With $\{\mu\} \equiv \{n\}$ this theorem forms the basis of Littlewood's "third method" of obtaining the separation of a plethysm.

To use this recursive method the right hand side of eqn (1.34) is calculated first and then various $\{\nu\}$ are tried, until a consistent set is found. The choice is rather difficult and an array of "principle part" theorems are used[20-22].

Special Cases: From the definition of plethysm we have that

$$\begin{aligned} &\{m\} \otimes \{n\} \supset \{mn\} \\ &\{m\} \otimes \{\mu\} \not\supset \{mn\} \qquad \{\mu\} \neq \{n\} \text{ and } (\mu) \text{ a partition of } n \end{aligned} \tag{1.36}$$

Generally

$$\{\lambda\} \otimes \{n\} \supset \{n\lambda_1, n\lambda_2, \cdots, n\lambda_r\} \tag{1.36a}$$

and this term, being the principal part of the n-fold product, does not occur in any other plethysm $\{\lambda\} \otimes \{\mu\}$. Likewise, in the n-fold product no S-function on greater than nr parts will occur.

Certain other special results can be obtained:

$$\begin{aligned} \{\lambda\} \otimes \{0\} &= \{0\} \\ \{\lambda\} \otimes \{1\} &= \{\lambda\} \\ \{n\} \otimes \{2\} &= \{2n\} + \{2n-2,2\} + \{2n-4,4\} + \cdots \\ \{n\} \otimes \{11\} &= \{2n-1,1\} + \{2n-3,3\} + \cdots \\ \{0\} \otimes \{\lambda\} &= \{0\} \quad \text{for } \{\lambda\} = \{n\} \\ &= 0 \text{ otherwise} \end{aligned} \tag{1.37}$$

$$\{1\} \otimes \{\lambda\} \;=\; \{\lambda\}$$

$\{2\} \otimes \{n\}$ = all S-functions corresponding to partitions of 2n into even parts only.

Two theorems due to F.D. Murnaghan[23,24] lead to a systematic evaluation of any plethysm. The method is still recursive, but does not lead to any arbitrary choices like the method above.

We use $[\{\lambda\}]_k$ to denote the result of subtracting one node from each row of the corresponding diagram (λ) of k parts, all other diagrams contribute nothing.

e.g. $[\{6\} + \{51\} + \{42\} + \{222\}]_2 \;=\; \{4\} + \{31\}$

The theorems state:

$$[\{m\}\otimes\{n\}]_k \;=\; \sum_{r=1}^{n-k} (-1)^{r-1}(\{m\}\otimes\{1^r\})[\{m\}\otimes\{n-r\}]_k$$

$$+\; (-1)^{n-k}(\{m-1\}\otimes\{1^n\})\{n-k\} \qquad (1.38)$$

$$[\{m\}\otimes\{1^n\}]_k \;=\; \sum_{r=1}^{n-k} (-1)^{r-1}(\{m\}\otimes\{r\})[\{m\}\otimes\{1^{n-r}\}]_k$$

$$+\; (-1)^{n-k}(\{m-1\}\otimes\{n\})\{n-k\} \qquad (1.39)$$

Where we omit all terms in the products that have more than k parts.

Using a table of $\{m\}\otimes\{n\}$ and $\{m\}\otimes\{1^n\}$ it is a straightforward, if lengthy, process to build up, using eqns

(1.27-1.32), any plethysm $\{\lambda\}\otimes\{\mu\}$ required. It will be noted that if $\{\lambda\}$ is on a relatively small number of variables, many S-functions that would otherwise occur, will be null. In this process of building up a plethysm it is easy to omit such terms when they first make their appearance.

It is by using this method that the table of plethysms in Appendix III was machine calculated.

9. INNER PLETHYSMS

At this point it is natural to introduce the concept of the symmetrized inner product[10,25,26] $\{\lambda\}\odot\{\mu\}$ where

$$\{\lambda\}\circ\{\lambda\}\circ\cdots n \text{ times} = \Sigma(f\{\mu\}).\{\lambda\}\odot\{\mu\} \qquad (1.40)$$

This operation has its similarities with outer plethysm

$$\{\lambda\} \odot (A\pm B) = \{\lambda\}\odot A \pm \{\lambda\}\odot B \qquad (1.41)$$

$$\{\lambda\} \odot (A.B) = (\{\lambda\}\odot A)\circ(\{\lambda\}\odot B) \qquad (1.42)$$

$$(A+B) \odot \{\lambda\} = \Sigma(A\odot\{\mu\}) \circ [B \odot (\{\lambda\}/\{\mu\})] \qquad (1.43)$$

$$(A-B) \odot \{\lambda\} = \Sigma(-1)^p[A \odot (\{\lambda\}/\{\mu\})] \circ (B\odot\{\tilde{\mu}\}) \qquad (1.44)$$

$$(\mu) \text{ a partition of } p$$

$$(A\circ B) \odot \{\lambda\} = \Sigma(A\odot\{\mu\}) \circ [B \odot (\{\mu\}\circ\{\lambda\})] \qquad (1.45)$$

It is to be noted that the operation behaves as an inner operation on the left and as an outer operation on the right, in particular

$$(\{\lambda\} \circledcirc \{\mu\}) \circledcirc \{\nu\} = \{\lambda\} \circledcirc (\{\mu\} \otimes \{\nu\}) \tag{1.46}$$

We have the dimension check

$$f(\{\lambda\} \circledcirc \{\mu\}) = \frac{f\{\mu\}}{n!} G^{\{\mu\}}(f(\{\lambda\})) \tag{1.47}$$

where

$$G^{\{\mu\}}(d) = \prod_{i=1}^{r} \prod_{j=1}^{\mu_i} (d + j - i) \tag{1.47a}$$

Littlewood[26] gives the special result that

$$\{m-1,1\} \circledcirc \{1^k\} = \{m-k,1^k\} \tag{1.48}$$

Several other special results follow from eqs (1.40) and (1.47).

Since $\{m\} \circ \{m\} \circ \cdots \circ \{m\} = \{m\}$

which by eqn (1.40) $= \Sigma f(\{\mu\}) \{m\} \circledcirc \{\mu\}$

we have $\{m\} \circledcirc \{\mu\} = 0$ unless $\{\mu\} = \{n\}$ or $\{1^n\}$

but $G^{\{1^n\}}(1) = 0 \quad n > 1$

$$\therefore \quad \{m\} \circledcirc \{n\} = \{m\} \tag{1.49a}$$

$$\text{and} \quad \{m\} \circledcirc \{\mu\} = 0 \quad \{\mu\} \neq \{n\} \tag{1.49b}$$

$$\text{Similarly} \quad \{1^m\} \circledcirc \{n\} = \{m\} \quad n \text{ even} \tag{1.50a}$$

$$= \{1^m\} \quad n \text{ odd}$$

$$\text{and} \quad \{1^m\} \circledcirc \{\mu\} = 0 \quad \{\mu\} \neq \{n\} \tag{1.50b}$$

And using eqn (1.45)

$$\{\tilde{\lambda}\} \odot \{\mu\} = (\{1^m\} \circ \{\lambda\}) \odot \{\mu\}$$

$$= \{\lambda\} \odot \{\mu\} \qquad n \text{ even} \qquad (1.51a)$$

$$= \widetilde{\{\lambda\} \odot \{\mu\}} \qquad n \text{ odd} \qquad (1.51b)$$

Since we know $\{m-1,1\} \odot \{1^k\}$ (eqn (1.48)) we may evaluate $\{m-1,1\} \odot \{\mu\}$ by expressing $\{\mu\}$ in terms of the $a_r \equiv \{1^r\}$. Using also eq.(1.46) we have

$$\{m-k,1^k\} \odot \{\mu\} = \{m-1,1\} \odot (\{1^k\} \otimes \{\mu\}). \qquad (1.52)$$

To evaluate $\{\lambda\} \odot \{\mu\}$, $\{\lambda\}$ not of the form $\{m-k,1^k\}$ presents a more difficult problem. A procedure similar to that for outer plethysms presents itself. We need only write a given S-function in terms of an inner product of functions of the form $\{m-k,1^k\}$.

e.g. $\{321\} = \{411\} \circ \{51\} - \{3111\} - \{411\} - \{42\} - \{51\}$

$\{42\} = \{51\} \circ \{51\} - \{411\} - \{51\} - \{6\}$

$\therefore \{321\} = \{411\} \circ \{51\} - \{51\} \circ \{51\} - \{3111\} + \{6\}$

and $\{33\} = \{42\} \circ \{51\} - \{321\} - \{411\} - \{42\} - \{51\}$

$\therefore \{33\} = \{51\} \circ \{51\} \circ \{51\} - 2\{411\} \circ \{51\} - \{51\} \circ \{51\}$

$- \{51\} + \{3111\}$

Theorem: It is always possible to write an S-function $\{\lambda\}$ in terms of d-fold inner products

$$\{\lambda\} \;=\; \Sigma \pm \{m-a,1^a\} \circ \{m-b,1^b\} \circ \{m-c,1^c\} \circ \cdots \circ \{m-d,1^d\} \tag{1.53}$$

To prove this, we define a new ordering among the S-functions $\{\lambda\}$, $\{\mu\}$, partitions of m, that differs from the usual ordering. We say $\{\lambda\}$ preceeds $\{\mu\}$ if,

(i) $\lambda_1 > \mu_1$

or if their first rows are equal, by the length of the first column:

(ii) $(\tilde{\lambda})_1 > (\tilde{\mu})_1$

If both first row and first column are equal we order with respect to the smallness of their lowest rows. $\lambda_r < \mu_r$

e.g. $\{421\} > \{43\} > \{3211\} > \{331\} > \{322\} > \{2^21^3\} > \{2^31\}$

We may replace $\{\lambda\}$, $\{\lambda\}$ not of the form $\{m-k,1^k\}$, by the set of S-functions given by

$$\{\lambda''\} \circ \{\mu\} - \Sigma\{\nu\} \tag{1.54}$$

where $\{\lambda''\} \circ \{\mu\} \;=\; \{\lambda\} + \Sigma\{\nu\}$ and we are to prove that all the terms $\{\lambda''\}$, $\{\mu\}$ and $\{\nu\}$ preceed $\{\lambda\}$ in the above ordering.

If $\{\lambda\} \;=\; \{\lambda_1,\lambda_2,\cdots,\lambda_r1^n\}$

and

$\lambda_r \;=\; a+1 \qquad a > 0$

we take $\{\lambda''\} = \{\lambda_1+a, \lambda_2, \cdots, \lambda_{r-1}, 1^{n+1}\}$

$\{\mu\} = \{m-a, a\}$

It is clear that both $\{\lambda''\}$ and $\{\mu\}$ preceed $\{\lambda\}$ in the ordering.

We may write

$$\{\mu\} = \{m-a\}\{a\} - \{m-a+1\}\{a-1\} \tag{1.55}$$

and by Eqn (1.20)

$$\{\lambda''\} \circ \{\mu\} = (\{\lambda''\}/\{\xi_a\})\{\xi_a\} - (\{\lambda''\}/\{\xi_{a-1}\})\{\xi_{a-1}\} \tag{1.56}$$

where $\{\xi_a\}$ is summed over all partitions of a. All terms $\{\lambda''\}/\{\xi_a\}$, $\{\lambda''\}/\{\xi_{a-1}\}$ will have at least λ_1+1 cells in the first row except one term of $\{\lambda''\}/\{a\}$. This one term of $\{\lambda''\}/\{a\}$ is $\{\lambda_1, \lambda_2, \cdots \lambda_{r-1}, 1^{n+1}\}$. All the $\{\nu\}$ arising from the products of the other terms with their respective $\{\xi\}$ must preceed $\{\lambda\}$ in our ordering on account of condition 1. One term in $\{\lambda_1, \lambda_2, \cdots, \lambda_{r-1}, 1^{n+1}\}\{a\} = \Sigma\{\nu\}$ is $\{\lambda\}$, all other terms will have $\nu_r < a+1$, i.e. $\nu_r < \lambda_r$ (condition 3). This proves that by use of eqn (1.52) we may systematically replace the lowest $\{\lambda\}$ in an inner product expression by terms "higher" in this ordering.

This method I have derived allows the systematic evaluation of any symmetrized inner product. It is clear that, like outer plethysms, there is much manipulation to be done for all but the simplest calculations.

e.g. $\{321\} \circledcirc \{11\} = (\{41^2\} \circ \{51\} - \{51\} \circ \{51\} - \{31^3\} + \{6\})$
$\circledcirc \{11\}$

by eqn (1.43-1.44)

$$
\begin{aligned}
= & (\{41^2\} \circ \{51\}) \circledcirc \{11\} + \{51\} \circ \{51\} \circledcirc \{2\} \\
& + \{31^3\} \circledcirc \{2\} + \{6\} \circledcirc \{11\} - \{41^2\} \circ \{51\} \\
& \circ \{51\} \circ \{51\} - \{411\} \circ \{51\} \circ \{31^3\} \\
& + \{41^2\} \circ \{51\} + \{51\} \circ \{51\} \circ \{31^3\} \\
& - \{51\} \circ \{51\} - \{31^3\}
\end{aligned}
$$

but we have also by eqn (1.45)

$$
\begin{aligned}
(\{41^2\} \circ \{51\}) \circledcirc \{11\} = & \{41^2\} \circledcirc \{2\} \circ \{51\} \circledcirc \{11\} \\
& + \{41^2\} \circledcirc \{11\} \circ \{51\} \circledcirc \{2\}
\end{aligned}
$$

and $(\{51\} \circ \{51\}) \circledcirc \{2\} = (\{51\} \circledcirc \{2\})^2 + (\{51\} \circledcirc \{11\})^2$

Use of eqs (1.41 - 1.42) and eqn (1.48) gives

$$\{51\} \circledcirc \{11\} = \{41^2\}$$

$$\{51\} \circledcirc \{2\} = \{51\} \circ \{51\} - \{41^2\}$$

Using also eqn (1.52) we also obtain

$$\{31^3\} \circledcirc \{2\} = \{41^2\} \circ \{41^2\} - \{51\} \circ \{41^2\} + \{51\}$$

and $\{41^2\} \circledcirc \{11\} = \{51\} \circ \{31^3\} - \{21^4\}$

$$\{41^2\} \circledcirc \{2\} = \{41^2\} \circ \{41^2\} - \{51\} \circ \{31^3\} + \{21^4\}$$

and finally using $\{6\} \circledcirc \{11\} = 0$ leads to the result:

$$\{321\} \odot \{11\} = 3\{41^2\} + \{3^2\} + 2\{321\} + 3\{31^3\} + 2\{2^21^2\} + \{21^4\}$$

verifying the result given by Robinson[10] by other means.

CHAPTER 2

GENERATING FUNCTIONS AND SPECIAL SERIES

1. INTRODUCTION

In Chapter 1 we defined S-functions in terms of variables $x_1, x_2, \cdots, x_n$ and we stated graphical and combinatorial methods of analysing various "products" of such functions. If we work with generating functions it is a straightforward matter to prove the various expansions, and Littlewood[7] in fact derives many of the results from this approach.

It is clear, by actually doing the multiplication, that the a_r's defined by:

$$f(x) \quad = \quad \prod_{i=1}^{n} (1-\alpha_i x) \quad = \quad \sum_{r=0}^{n} (-1)^r \, a_r x^r \quad = \quad 0 \qquad (2.1)$$

are the elementary symmetric functions $\{1^r\}$ defined earlier.

Likewise:

$$1/f(x) \quad = \quad \prod_{i=1}^{n} (1-\alpha_r x)^{-1} \qquad (2.2)$$

$$= \quad \sum_{r=0}^{\infty} h_r x^r \qquad (2.3)$$

and where $h_r = \{r\}$.

Much work in the last century was put into discovering the properties of these and other symmetric functions. However, for our purposes it is sufficient to quote several results of such analysis. The S-function itself was not defined until much later but the properties of the bialternant

$$\{\lambda\} = \frac{|\alpha_s^{\lambda_t+n-t}|}{|\alpha_s^{n-t}|} \tag{2.4}$$

were also extensively studied, and the result obtained

$$\{\lambda\} = \frac{|\alpha_s^{\lambda_t+n-t}|}{|\alpha_s^{n-t}|} = |h_{\lambda_s-s+t}| = |a_{\mu_s-s+t}| \tag{2.5}$$

where $\{\mu\} = \{\tilde{\lambda}\}$.

It is usual to write

$$\Delta(\alpha_1,\cdots\alpha_n) = \pi_{i<j} (\alpha_i - \alpha_j) \tag{2.6}$$

Various other relations may be derived. In particular we may show that any symmetric function $\Sigma\alpha_1^{a_1}\cdots\alpha_r^{a_r}$ with $a_1+\cdots+a_p = p$ may be re-expressed in the form $\Sigma K_{(\lambda)}\{\lambda\}$, (λ) a partition of p.

2. GENERALIZED DEFINITION OF THE S-FUNCTION

When we defined the S-function in Chapter I we wrote

$$\{\lambda\} = |h_{\lambda_s-s+t}|$$

It is convenient to retain this definition for the case of $\{\lambda\}$ not being of the form $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_r$. Any $\{\lambda\}$

not of this form may be expressed as such by simply interchanging adjacent rows of the determinant, leading to

$$\{\lambda_1,\cdots,\lambda_{i-1},\lambda_i,\lambda_{i+1},\lambda_{i+2},\cdots,\lambda_r\}$$

$$= -\{\lambda_1,\cdots,\lambda_{i-1},\lambda_{i+1}-1,\lambda_i+1,\lambda_{i+2},\cdots,\lambda_r\} \qquad (2.7)$$

The generating functions of a_r and h_r may be re-expressed

$$f(x) = \pi(1-\alpha_r x) = 1 - \{1\}x + \{1^2\}x^2 - \cdots + (-1)^r\{1^r\}x^r + \cdots \qquad (2.1a)$$

$$F(x) = 1/\pi(1-\alpha_r x) = 1 + \{1\}x + \{2\}x^2 + \cdots + \{r\}x^r + \cdots \qquad (2.2a)$$

and these generating relations may be generalized to give the generating function for S-functions on p variables

$$\pi_{r=1}^{p} F(x_r)\Delta(x_1,x_2\cdots x_p) = \Sigma \pm \{\lambda\}\, x_1^{\lambda_1+p-1}\, x_2^{\lambda_2+p-2} \cdots x_p^{\lambda_p} \qquad (2.8)$$

where $F(x_r)$ are p functions with the roots $\alpha_1\cdots\alpha_n$, and the sum is over all $\{\lambda\}$ and all permutations of the suffixes, the minus sign being taken for an odd permutation.

The S-function $\{\lambda\}$ is on the roots α of $F(x) = 0$. Denoting an S-function on the variables $x_1\cdots x_n$ by $\{x;\lambda\}$ we have, analogous to the expansion of eqn (2.5) that

$$\Sigma \pm x_1^{\lambda_1+p-1}\, x_2^{\lambda_2+p-2} \cdots x_p^{\lambda_p} = \{x;\lambda\}\Delta(x_1\cdots x_p). \qquad (2.9)$$

Eqn (2.8) leads to

$$\pi F(x_r)\Delta(x_1\cdots x_p) = [\Sigma\{\lambda\}\{x;\lambda\}]\Delta(x_1\cdots x_p)$$

$$\therefore \quad \pi F(x_r) = \Sigma\{\lambda\}\{x;\lambda\}$$

$$\text{i.e. } \pi F(x_r)_s \equiv 1/\underset{r,s}{\pi}(1-\alpha_s x_r) = \Sigma\{\alpha;\lambda\}\{x;\lambda\} \tag{2.10}$$

3. SPECIAL SERIES OF S-FUNCTIONS

For the calculation of group characters in the next chapter, we shall require expansions of certain symmetric functions of the variables $\alpha_1\cdots\alpha_n$, in terms of the S-functions associated with these variables. We shall need

$$\pi(1-\alpha_i\alpha_j) = \Sigma(-1)^{\frac{1}{2}p}\{\alpha\} \qquad \text{(i)}$$

$$1/\pi(1-\alpha_i\alpha_j) = \Sigma\{\beta\} \qquad \text{(ii)}$$

$$\pi(1-\alpha_i^2)\pi(1-\alpha_i\alpha_j) = \Sigma(-1)^{\frac{1}{2}p}\{\gamma\} \qquad \text{(iii)}$$

$$1/\pi(1-\alpha_i^2)\pi(1-\alpha_i\alpha_j) = \Sigma\{\delta\} \qquad \text{(iv)}$$

$$\pi(1-\theta\alpha_i)\pi(1-\alpha_i\alpha_j) = \Sigma\theta^p(-1)^{\frac{1}{2}(p+r)}\{\varepsilon\} \qquad \text{(v) \& (vii)}$$

$$1/\pi(1-\theta\alpha_i)\pi(1-\alpha_i\alpha_j) = \Sigma\theta^p\{\eta\} \qquad \text{(vi) \& (viii)}$$

(2.11)

where the S-functions are partitions of p into r parts. The sequences are as follows:

$\{\lambda\}$: all partitions which in Frobenius notation are of the form $\binom{a}{a+1}, \binom{a \quad b}{a+1 \quad b+1}, \binom{a \quad b \quad c}{a+1 \quad b+1 \quad c+1}, \cdots$

$\{\beta\}$: all partitions which have an even number of parts of any given magnitude.

$\{\gamma\}$: the conjugate series to $\{\alpha\}$, i.e. those of the form

$$\binom{a+1}{a}, \binom{a+1 \quad b+1}{a \quad b},$$

$\{\delta\}$: the conjugate series to β, i.e. partitions into even parts only

$\{\varepsilon\}$: all self-conjugate partitions.

$\{\eta\}$: all S-functions.

When we include the phase factors the series are

$$\{0\} - \{11\} + \{211\} - \{31^3\} + \{2^3\} + \{41^4\} + \{32^21\} - \quad \text{(i)}$$

$$\{0\} + \{11\} + \{2^2\} + \{1^4\} + \{2^21^2\} + \{3^2\} + \{1^6\} + \{4^2\} + \cdots \quad \text{(ii)}$$

$$\{0\} - \{2\} + \{31\} - \{411\} - \{3^2\} + \{51^3\} + \{431\} - \quad \text{(iii)}$$

$$\{0\} + \{2\} + \{4\} + \{22\} + \{6\} + \{42\} + \{222\} + \cdots \quad \text{(iv)}$$

$$\{0\} - \{1\} + \{21\} - \{22\} - \{31^2\} + \{321\} + \{41^3\} - \{3^22\} - \{421^2\} \quad \text{(v)}$$

$$\{0\} + \{1\} + \{2\} + \{11\} + \{3\} + \{21\} + \{111\} + \{4\} + \cdots \quad \text{(vi)}$$

$$\{0\} + \{1\} - \{21\} - \{22\} + \{31^2\} + \{321\} - \{41^3\} - \{3^22\} - \{421^2\} \quad \text{(vii)}$$

$\{0\} - \{1\} + \{2\} + \{11\} - \{3\} - \{21\} - \{111\} + \{4\} + \cdots$ (viii)

It is readily verified that the four pairs, (i) & (ii), (iii) & (iv), etc., when multiplied together, give $\{0\}$, as is required by their definition.

Littlewood[7] derives these expansions, except (vi) and (viii). These two may be derived by similar methods.

C H A P T E R 3

CHARACTER THEORY OF THE CONTINUOUS GROUPS

This chapter is devoted to an analysis of the properties of characters of the continuous groups. I first rederive the expression of these characters in terms of S-functions correcting some errors in previous works (sections 1-8). Most of these results, although well known[7], are not generally used by physicists. The remainder of the chapter uses the powerful tools of S-functional analysis to give systematic prescriptions for the calculation of all branching rules, Kronecker products and selection rules for compact representations of the Cartan classes of groups A_n, B_n, C_n and D_n, also for the exceptional group G_2. Given the expression of the other exceptional group characters, in terms of S-functions, their properties would also follow immediately by these methods.

1. EXTENSION OF FINITE GROUP PROPERTIES TO UNITARY MATRICES

The set of all n x n matrices with non-zero determinant satisfy the group axioms. To extend the orthogonal properties of group characters to such a group, the summation over the group elements must be replaced by integration over the group manifold.

If we require that the group manifold be a closed finite space, we are led to the condition that the characteristic roots of the matrices have unit modulus. Such a compact group, is most generally, the group of unitary matrices of order n x n. That is, U_n.

Each element a_{ij} of a unitary matrix is algebraically independent of its complex conjugate a^*_{ij}. The n^2 elements of the matrix have n^2 orthonormality relations between them:

$$\sum_r a_{r_i} a^*_{r_j} = \delta_{ij} \tag{3.1}$$

and thus the n^2 elements are linearly independent. Thus[7] every algebraic invariant of the group of unitary matrices is also an invariant of the group of all non-singular real matrices GL(n). But in the previous chapter we showed that all such invariants can be expressed as S-functions.

Hence we may show that the complete set of characters of U_n are the S-functions of the characteristic roots. It is worth remarking that since each characteristic root has modulus unity, the n complex numbers which are the roots, require only one parameter, and thus the S-functions are on n independent variables of the form $e^{i\phi_r}$.

2. INTEGRATION OVER THE UNITARY GROUP MANIFOLD

A matrix of an infinitesimal transformation may be written $I + \Phi$ where Φ is a skew-Hermitian matrix with infinitesimal elements ϕ_{ij}.

We have

$$\phi_{pp} = i\phi''_{pp} \tag{3.2a}$$

$$\phi_{pq} = \phi'_{pq} + i\phi''_{pq} \qquad p \neq q \tag{3.2b}$$

When each real parameter ϕ''_{pp}, ϕ'_{pq}, ϕ''_{pq}, $p < q$ varies independently and continuously between the limits 0 and ϕ''_{pp}, ϕ'_{pq}, ϕ''_{pq} respectively, we define a volume content of this subspace of the group manifold as

$$|\Phi| = |\pi\phi''_{pp} \prod_{p<q} \phi'_{pq}\phi''_{pq}|. \tag{3.3}$$

When Φ is transformed by a unitary matrix the volume content will be unaltered

$$|S^{-1}\Phi S| = |\Phi| \tag{3.4}$$

Thus volume content of the space described by $S+dS$ is

$$|dS| = |S^{-1}dS| \tag{3.5}$$

since $|S^{-1}dS|$ is the volume content of $|\Phi|$ in the neighbourhood of the identity. This leads to the volume content of the complete group manifold as

$$g = \int |dS| \equiv \int dS \tag{3.6}$$

and for any function of the group elements

$$\int x(S)\,dS = \int x(TS)\,dS = \int x(TSU)\,dS$$

where T and U are any matrices of the group.

From the definition of a class of conjugate elements we have for a class function x that

$$x(S) = x(A^{-1}SA) \tag{3.7}$$

and we may thus choose A such that $A^{-1}SA = D = \text{diag}\,(e^{i\phi_1}, e^{i\phi_2},\cdots,e^{i\phi_n})$. The class function becomes

$$x(S) = x(D) = f(\phi_1,\phi_2\cdots\phi_n) \tag{3.7a}$$

By a similar change of parameters of dS we are led to

$$\int f(\phi)\,dS = K\int_0^{2\pi}\cdots\int_0^{2\pi} f(\phi)\,\Delta(e^{i\phi_r})\,\Delta(e^{-i\phi_r})\,d\phi_1\cdots d\phi_n \tag{3.8}$$

where the $\Delta(\alpha_r)$ is the antisymmetric function (2.6) and K may be evaluated by putting $f(\phi) = 1$.

3. THE ORTHOGONAL GROUP MANIFOLDS

Real orthogonal matrices have determinant ±1 and form a real subgroup of the unitary group. The canonical form of S can be of four types, depending on the sign of the determinant and depending on whether n is even or odd.

$n = 2\nu$

a) $$D_1 = \text{diag}\,(\Phi_1,\Phi_2\cdots\Phi_\nu) \tag{3.9a}$$

b) $$D_2 = \text{diag}\,(1,-1,\Phi_1\cdots\Phi_{\nu-1}) \tag{3.9b}$$

$n = 2\nu+1$

c) $D_3 = \text{diag}\ (1, \Phi_1, \Phi_2 \cdots \Phi_\nu)$ (3.9c)

d) $D_4 = \text{diag}\ (-1, \Phi \cdots \Phi_\nu)$ (3.9d)

$$\text{where } \Phi_r = \begin{pmatrix} \cos\phi_r & \sin\phi_r \\ -\sin\phi_r & \cos\phi_r \end{pmatrix} \tag{3.10}$$

By methods similar to the previous section, we obtain the respective integration formulae for class functions, $f(\phi)$:

a) $\int f(\phi)\,dS = K_a \int \cdots \int f(\phi)\Delta^2(\cos\phi_r)\ d\phi_1 \cdots d\phi_\nu$

b) $\int f(\phi)\,dS = K_b \int \cdots \int f(\phi)\ \pi(\sin^2\phi_r)\Delta^2(\cos\phi_r)\ d\phi_1 \cdots d\phi_{\nu-1}$

c) $\int f(\phi)\,dS = K_c \int \cdots \int f(\phi)\ \pi(1-\cos\phi_r)\Delta^2(\cos\phi_r)\ d\phi_1 \cdots d\phi_\nu$

d) $\int f(\phi)\,dS = K_d \int \cdots \int f(\phi)\ \pi(1+\cos\phi_r)\Delta^2(\cos\phi_r)\, d\phi_1 \cdots d\phi_\nu$

(3.11)

4. THE CHARACTERS OF THE UNITARY GROUP

At the beginning of this chapter we showed that the S-functions on the characteristic roots $\alpha_r \equiv e^{i\phi_r}$ of the matrices were characters of the unitary group. For these to be simple (irreducible) characters we must have

$$\frac{1}{g} \int \{\lambda\}\{\mu\}^* dS = \delta_{(\lambda)(\mu)} \tag{3.12}$$

where $\{\mu\}^*$ denotes the complex conjugate of $\{\mu\}$.

Now $\quad \{\lambda\}\,\Delta\,(\alpha_r) \quad = \quad \left|\alpha_s^{\lambda_t+n-t}\right|$ (2.4)

and $\quad \alpha_r^* \quad = \quad \alpha_r^{-1}$

thus

$$\int\cdots\int\{\lambda\}\{\mu\}^*\Delta(\alpha_r)\Delta(\alpha_r^*)\,d\phi_1\cdots d\phi_n$$

$$= \int\cdots\int\left|\alpha_s^{\lambda_t+n-t}\right|\cdot\left|\alpha_s^{-\mu_t-n+t}\right|\,d\phi_1\cdots d\phi_n$$

$$= 0 \qquad (\lambda) \neq (\mu)$$

$$= n!(2\pi)^n \qquad (\lambda) = (\mu) \qquad (3.13)$$

by expanding out the determinants as sums and products. By setting $\{\lambda\} = \{\mu\} = 1$ we note that $g = n!(2\pi)^n$, and thus all S-functions $\{\alpha;\lambda\}$ are the simple characters of U_n.

5. CLASS FUNCTIONS OF THE ORTHOGONAL AND ROTATION GROUPS

We denote the group O_n of orthogonal matrices T by D'. The subgroup R_n of matrices S of positive determinant we denote by D. The set of remaining matrices U we denote by D_1. They do not form a group.

For integration over the O_n manifold we have

$$\int x(T)\,dT \quad = \quad \int x(S)\,dS + \int x(U)\,dU \qquad (3.14)$$

If for U_1, a fixed element of D_1, we have $U_1S \supset D_1$ and $U_1U \supset D$, then we would have

$$\int dU \;=\; \int dS \;=\; h; \qquad \int dT \;=\; 2h \qquad (3.15)$$

For the case of odd n, $n = 2\nu+1$, there are such elements, e.g. $-I$. If two matrices S_1 and S_2 are equivalent in D' then they will also be equivalent in D, for if

$$S_2 \;=\; U^{-1}S_1 U$$

then $$S_2 \;=\; (U\,U_1)^{-1}\, S_1(U\,U_1)$$

where $$U_1 \;=\; -I \quad \text{and} \quad U\,U_1 \supset D.$$

Thus the same parameters may be used for the two matrices U and S.

For the case of even n, there is no such element U_1, since $-I \supset D$, and one class in D' may in general separate into two conjugate classes in D. For $n = 4r$, S and S^{-1} will belong to the same class but for $n = 4r+2$, S and S^{-1} belong to conjugate classes.

All class functions of $D(2n+1)$ are unchanged by setting $\phi_r = -\phi_r$. Not all class functions of $D(2\nu)$ have this property of being an even class function. Those which do take the same value for both D and D_1 and are therefore also class functions of D'.

If $\chi(T)$ is a simple character of D' we have

$$\int \chi(T)^2 dT \;=\; 2h \;=\; \int \chi(S)^2 dS + \int \chi(U)^2 dU. \qquad (3.16)$$

This leads to the possibilities that $\chi(S)$ is either a simple character of D, or a sum of two, when it is said to be a double character of D', and these have $\chi(U) = 0$, resulting in:

a) If $n = 2\nu+1$ all the simple characters of D' are simple characters of D.

b) If $n = 4r+2$ all the double characters of D' are the sum of two complex conjugate characters of D.

c) If $n = 4r$ all characters of D are real.

6. THE CHARACTERS OF THE ORTHOGONAL GROUP

Using the integration formulae and with some algebraic manipulation Littlewood is able to show that

$$[\lambda]' = |q_{\lambda_s-s+1}, q_{\lambda_s-s} + q_{\lambda_s-s+2}, \cdots, q_{\lambda_s-s-v+2} + q_{\lambda_s-s+v}| \tag{3.17}$$

is a simple character of O_n where q_r is associated with the series

$$\frac{1-x^2}{f(x)} = \Sigma\, q_r\, x^r$$

and $f(x) = 0$ is the characteristic equation of the matrices. We have also that

$$L(x)\pi \frac{1-x_i^2}{f(x_i)} = \Sigma[\lambda]\{x;\lambda\} \tag{3.18}$$

where $L(x) = \pi(1-x_i x_j)$

Now $$1/\pi f(x) = \Sigma\{\lambda\}\{x;\lambda\} \qquad (2.10)$$

and $$L(x)\pi(1-x_i^{\,2}) = \Sigma(-1)^{\frac{1}{2}p}\{x;\gamma\} \qquad (2.11.iii)$$

By comparing coefficients

$$[\lambda]' = \Sigma(-1)^{\frac{1}{2}p}\Gamma_{\nu\gamma\lambda}\{\nu\} \equiv \{\lambda\}/(-1)^{\frac{1}{2}p}\{\gamma\} \qquad (3.19)$$

The inverse relation follows

$$\{\lambda\} = [\{\lambda\}/\{\delta\}]' \qquad (3.20)$$

where the S-functions on the right are taken as characters of O_n.

The characters of the orthogonal group may be expressed in terms of S-functions on only the variable roots. Table I gives the results for the four types of matrix and also the usual determinantal form of the characters.

7. THE CHARACTERS OF THE ROTATION GROUP

We showed in section 5 that:
for n odd, the characters of R_n are just those of O_n;
for n even, if $[\lambda]'$ is not a double character then

$$[\lambda]' \to [\lambda] + [\lambda'] \qquad (3.21)$$

We define the difference character of $R_{2\nu}$ as

$$[\lambda]'' = [\lambda] - [\lambda'] \qquad (3.22)$$

It is relatively easy to show that the difference character

TABLE I: Alternative Forms of the Characters of O_n

$n = 2\nu$

For matrix S of determinant +1

$$[\lambda]' = \{\lambda\}/(-1)^{\frac{1}{2}p}\{\gamma\} = \frac{|C_t^{(\lambda_s+\nu-s)}|}{|C_t^{(\nu-s)}|}$$

matrix U, determinant = -1

$$[\lambda]' = \{\lambda\}/(-1)^{\frac{1}{2}p}\{\alpha\} = \frac{|S_t^{(\lambda_s+\nu-s+1)}|}{|S_t^{(\nu-s+1)}|}$$

$n = 2\nu+1$

For matrix S determinant $\Theta = \pm 1$

$$[\lambda]' = \{\lambda\}/(-)^{\frac{1}{2}(p+r)}(-\Theta)^p\{\eta\}.$$

$$\Theta = +1,\ [\lambda]' = \frac{|S_t^{(\lambda_t+\nu-s+\frac{1}{2})}|}{|S_t^{(\nu-s+\frac{1}{2})}|}$$

$$\Theta = -1,\ [\lambda]' = \frac{|C_t^{(\lambda_t+\nu-s+\frac{1}{2})}|}{|C_t^{(\nu-s+\frac{1}{2})}|}$$

where $S_i^{(j)} = 2\sin(j\phi_i)$

$C_i^{(j)} = 2\cos(j\phi_i)$ and where the S-functions are on the variable characteristic roots only.

is given by

$$[\lambda]'' \equiv [\mu_1+1,\mu_2+1,\cdots,\mu_\nu+1] = \Delta_1(\{\lambda\}/(-1)^{\frac{1}{2}p}\{\alpha\}) \quad (3.24)$$

where Δ_1 is the simple difference character given by:

$$\Delta_1 = [1^\nu]'' = \pi(2i \sin \phi_r) \quad (3.25)$$

The integration required is carried out by a change of variables to use the integration results of eqs (3.11) and Table I.

8. SPIN REPRESENTATIONS

For the orthogonal and rotation groups, for all n, there exist so called p-valued representations of the group, by which each group element is represented by p matrices (see for example[7], p.249). Now, strictly, representations are by definition single valued - no more than one representation matrix for every group element - but for the above groups it is possible to have non-trivial two valued representations. Such representations are known as spin representations. The characters of spin representations of the orthogonal group, may be given as a product of a basic spin representation:

$$\Delta_{\frac{1}{2}} = [(\tfrac{1}{2})^\nu]' = \pi(2 \cos \tfrac{1}{2}\phi_r) \quad (3.26)$$

and a sum of sum S-functions.

$$[\lambda]' \equiv [\mu_1+\tfrac{1}{2},\mu_2+\tfrac{1}{2},\cdots,\mu_\nu+\tfrac{1}{2}]' = \Delta_{\frac{1}{2}}(\{\mu\}/(-1)^{\frac{1}{2}(p+r)}\{\varepsilon\}) \tag{3.27}$$

where we label representations by a series of ν half integral numbers. With this notation, the determinantal form of the spin character is the same as the expression for true representations as given in Table I.

I have derived the spin characters of the rotation group by an extension of the previous methods. To do this we require a basic spin difference character

$$\Delta''_{\frac{1}{2}} = [(\tfrac{1}{2})^{\nu}] - [(\tfrac{1}{2})^{\nu-1},-\tfrac{1}{2}] = \pi(2i \sin \tfrac{1}{2}\phi_r) \tag{3.27a}$$

These results are given in Table II.

9. BRANCHING RULES

The inverse S-functions series may be used for finding the branching rules for the representations of the unitary group to its subgroup.

Two other sub-groups are also of interest.

The Symplectic Group: Sp_n maintains invariant an anti-symmetric bilinear form. The expression of its characters in terms of the unitary group is

$$\langle\lambda\rangle = \{\lambda\}/(-1)^{\frac{1}{2}p}\{\alpha\} \tag{3.28}$$

The branching rule follows.

TABLE IIa: Characters of the Rotation Group expressed in terms of S-functions associated with the characteristic equation

$$f(x) = 0; \qquad 1/f(x) = \Sigma\{h_r\}x^r.$$

n = 2ν+1

true: $[\lambda] = \{\lambda\}/(-1)^{\frac{1}{2}p}\{\gamma\}$

spin: $[\lambda] \equiv [\mu+\frac{1}{2}] = \Delta_{\frac{1}{2}}\{\mu\}/(-1)^{\frac{1}{2}(p+r)}\{\varepsilon\}$

n = 2ν

true: $[\lambda] = [\mu+1] = \frac{1}{2}(\{\lambda\}/(-1)^{\frac{1}{2}p}\{\gamma\} + \Delta_1\{\mu\}/(-1)^{\frac{1}{2}p}\{\alpha\})$

$[\lambda'] \equiv [\lambda_1,\lambda_2,\cdots,\lambda_{\nu-1},-\lambda_\nu]$ = as above with negative sign.

spin: $[\lambda] = [\mu+\frac{1}{2}] = \frac{1}{2}(\Delta_{\frac{1}{2}}\{\mu\}/(-1)^{\frac{1}{2}(p+r)}\{\varepsilon\}$

$+ \Delta''_{\frac{1}{2}}\{\mu\}/(-1)^{\frac{1}{2}(p+r)}(-1)^p\{\varepsilon\})$

$[\lambda']$ as above.

where $\Delta_{\frac{1}{2}} = \pi(2\cos\frac{1}{2}\phi)$ $\qquad f(\Delta_{\frac{1}{2}}) = 2^\nu$

$\Delta''_{\frac{1}{2}} = \pi(2i\sin\frac{1}{2}\phi)$ $\qquad f(\Delta''_{\frac{1}{2}}) = 0$

$\Delta_1 = \pi(2i\sin\phi)$ $\qquad f(\Delta_1) = 0$

TABLE IIb: Characters of Rotation Groups in Determinantal Form.

n = 2ν+1

$$[\lambda] = \frac{|S_t^{(\lambda_s+\nu-s+\frac{1}{2})}|}{|S_t^{(\nu-s+\frac{1}{2})}|}$$

n = 2ν

$$[\lambda] = \tfrac{1}{2}([\lambda]' \pm [\lambda''])$$

$$[\lambda]' = \frac{|C_t^{(\lambda_s+\nu-s)}|}{|C_t^{(\nu-s)}|}$$

and $$[\lambda]'' = (i)^{\nu} \frac{|S_t^{(\lambda_s+\nu-s)}|}{|C_t^{(\nu-s)}|}$$

where $$S_i^{(j)} = 2 \sin (j\phi_i)$$

$$C_i^{(j)} = 2 \cos (j\phi_i)$$

The Exceptional Group G_2: The group G_2 is a proper subgroup of the seven dimensional rotation group and Judd[27] has derived the branching rules by using the infinitesimal operator approach, to yield the result

$$[\omega_1\omega_2\omega_3] \rightarrow \Sigma(i-k,j+k) + (j-k-1,i-j) \qquad (3.29)$$

where the sum is over all integral values of i, j, k satisfying the relations:

$$\omega_1 \geqslant i \geqslant \omega_2 \geqslant j \geqslant \omega_3 \geqslant k > -\omega_3.$$

The relation

$$(u_1u_2) = -(u_2-1,u_1+1)$$

is used to remove characters which do not give regular representations of G_2.

Such branching rules are not known for the other exceptional groups.

10. DIMENSIONS OF REPRESENTATIONS

The dimension of a representation is given by the character of the identity element, whose characteristic roots are all unity. Dimensions for various groups are given in Table III.

TABLE III: Dimensions of Representations of Groups

The Unitary Group U_n

$$f\{\lambda\} = \prod_{j>i=1}^{n} \frac{(j-i+\lambda_i-\lambda_j)}{(j-i)},$$

The Symplectic Group Sp_n, $n = 2\nu$

$$f\langle\lambda\rangle = \prod_{i=1}^{\nu} \frac{\lambda_i+\nu-i+1}{\nu-i+1} \prod_{j>i=1}^{\nu} (\lambda_i-\lambda_j+j-1)(\lambda_i+\lambda_j+2\nu+2-i-j).$$

The Orthogonal and Rotation Groups O_n, R_n

a) For odd dimensions $n = 2\nu+1$

$$f[\lambda] = \prod_{i=1}^{\nu} \frac{(2\lambda_i+n-2i)}{(n-2i)!} \prod_{i>j}^{\nu} (\lambda_i-\lambda_j+j-i)(\lambda_i+\lambda_j+n-i-j).$$

b) For even dimensions $n = 2\nu$

$$f[\lambda] = 2^{\nu-1} \prod_{i=1}^{\nu} \frac{1}{(2i-2)!} \prod_{i>j}^{\nu} (\lambda_i-\lambda_j-i+j)(\lambda_i+\lambda_j+n-i-j),$$

except that for the orthogonal group in the case of $\lambda_\nu \neq 0$ when the dimension is twice the above.

TABLE III (contd)

The Exceptional Group G_2

$$f(u_1u_2) = (u_1+u_2+3)(u_1+2)(2u_1+u_2+5)(u_1+2u_2+4)$$

$$\times (u_1-u_2+1)(u_2+1)/120.$$

11. NON-STANDARD SYMBOLS

Under the restriction of U_n to its subgroups O_n, R_n and Sp_n, we have relations between pairs of characteristic roots of the representation matrices. Any S-function on the roots is thus expressible in terms of S-functions not having more than ν parts. If we reduce the number of parts before applying the branching rules, we need never produce non-standard symbols in the subgroup characters. The problem of standardizing non-standard symbols has troubled many mathematicians. Littlewood's method is to write an S-function of more than ν parts in the form

$$\{r+\lambda_1, r+\lambda_2, \cdots, r+\lambda_\nu, r-\mu_\nu, r-\mu_{\nu-1}, \cdots, r-\mu_1\} \tag{3.30a}$$

if $n = 2\nu$, or in the form

$$\{r+\lambda_1, r+\lambda_2, \cdots, r+\lambda_\nu, r, r-\mu_\nu, r-\mu_{\nu-1}, \cdots, r-\mu_1\} \tag{3.30b}$$

if $n = 2\nu+1$.

Ignoring a possible change of sign for some transformations this S-function is independent of r and will be denoted $\{\lambda:\mu\}$. It is expanded to give a series of S-functions using the relation

$$\{\lambda:\mu\} = \Sigma(-1)^p(\{\lambda\}/\{\alpha\})(\{\mu\}/\{\tilde{\alpha}\}) \tag{3.31}$$

where the sum is over all S-functions $\{\alpha\}$, being partitions of p. This relation is used as often as necessary to reduce all terms to those of no more than ν parts.

Two special cases of this equivalence relation are often useful. In n variables for unitary transformations we have

$$\{\lambda\} = \{\lambda_1-\lambda_n,\lambda_2-\lambda_n,\cdots,0\}. \qquad (3.32)$$

Ignoring the change of sign when $n = 2\nu$ and then with transformations of negative determinant we have also

$$\{\lambda\} = \{\lambda_1-\lambda_n,\lambda_1-\lambda_{n-1},\cdots,0\}. \qquad (3.33)$$

This latter relation gives the well known particle-hole correspondence.

12. KRONECKER PRODUCTS FOR THE CONTINUOUS GROUPS

We may express the characters of the unitary and symplectic groups, and the characters of the true representations of the orthogonal group, in terms of S-functions. This means we may calculate the Kronecker products, in a straightforward manner, using directly the properties of the S-functions. The odd dimensional rotation groups follow in the same manner. I have calculated Kronecker products for G_2 in a similar manner, by a two stage process - express the characters of G_2 in terms of those of R_7, thence into S-functions. The expression of the characters of G_2 in terms of those of R_7

is performed by noting that in the reduction $R_7 \to G$, $[u_1u_2 0]$ contains (u_1u_2) as the term of highest weight. The terms of lower weights may be systematically removed by subtraction.

For example, in the case of (21) we may derive

$$[210] \to (11) + (20) + (21)$$

$$[200] \to (20)$$

$$[110] \to (11) + (10)$$

hence $$(21) = [210] = [200] - [110] + [100]$$

which may be expressed in S-functions to give

$$(21) = \{21\} - \{2\} - \{11\} + \{0\}.$$

Even Dimensional Rotation Groups: For even dimensional rotation groups, products in only two groups may be calculated directly, the groups in four and six dimensions. In six dimensions Littlewood[28] has shown that the group is isomorphic with the four dimensional full linear group and the correspondences

$$[abc] \leftrightarrow \{a+b, a-c, b-c\} \tag{3.34a}$$

$$\{pqrs\} \leftrightarrow [\tfrac{1}{2}(p+q-r-s), (p-q+r-s), \tfrac{1}{2}(p-q-r+s)] \tag{3.34b}$$

may be established, thus allowing us to perform the products easily. For the four dimensional rotation group there is a 2:1 homomorphism with the double binary full linear group and the correspondences

$$[a,b] \leftrightarrow \{a+b\}\{a-b\}' \tag{3.35a}$$

$$\{p\}\{q\}' \leftrightarrow [\tfrac{1}{2}(p+q),\tfrac{1}{2}(p-q)] \tag{3.35b}$$

may be made.

We may readily deduce that the separation of the Kronecker product in R_4 is given by

$$[a,b][c,d] = \sum_{\alpha=0}^{s} \sum_{\beta=0}^{t} [a+c-\alpha-\beta, b+d-\alpha+\beta] \tag{3.36}$$

where s is the lesser of (a+b) and (c+d) and t is the lesser of (a-b) and (c-d).

These homomorphisms are also valid for spin representations.

For spin representations of other orthogonal groups, and all representations of other even dimensional rotation groups we shall need to know more about the basic characters Δ_1, $\Delta_{\frac{1}{2}}$ and $\Delta''_{\frac{1}{2}}$.

When calculating the properties of a rotation character, true or spin, we express it in the form:

$$[\lambda] = \delta_a(\Sigma\{\mu\}) + \delta_b(\Sigma\{\nu\}) \tag{3.37}$$

where δ_a, δ_b are either 1 and Δ_1, or $\Delta_{\frac{1}{2}}$ and $\Delta''_{\frac{1}{2}}$. To calculate the Kronecker product of any representation with any other, we need to know the six products $\delta_a\delta_b$. It is clear that the product of two spin characters yields a true character, and a spin with a true yields a spin, etc.

n = 2ν+1: We consider first the orthogonal and rotation spin-characters in an odd dimensional group. There are no difference characters and Littlewood gives the square of the basic spin representation as

$$(\Delta_{\frac{1}{2}})^2 = \sum_0^{\nu} \{1^r\}. \tag{3.38}$$

n = 2ν: For the even dimensional groups we derive the results

$$\begin{aligned}
(\Delta_{\frac{1}{2}})^2 &= \Pi(2 \cos \tfrac{1}{2}\phi_r)^2 \\
&= \Pi(e^{i\frac{1}{2}\phi_r} + e^{-i\frac{1}{2}\phi_r})^2 \\
&= \Pi(e^{i\phi_r} + 2 + e^{-i\phi_r}) \\
&= \Pi(1 + e^{i\phi})(1 + e^{-i\phi}) \\
&= \sum_0^{2\nu} \{1^r\} \\
&= \{1^\nu\} + 2 \sum_0^{\nu-1} \{1^r\}
\end{aligned} \tag{3.39}$$

$$\begin{aligned}
(\Delta''_{\frac{1}{2}})^2 &= \Pi(2i \sin \tfrac{1}{2}\phi_r)^2 \\
&= \Pi(e^{i\frac{1}{2}\phi_r} - e^{-i\frac{1}{2}\phi_r})^2 \\
&= \Pi(e^{i\phi_r} - 2 + e^{-i\phi_r}) \\
&= \Pi[-(1 - e^{i\phi})(1 - e^{-i\phi})]
\end{aligned}$$

$$= (-1)^{\nu} \sum_{0}^{2\nu} (-1)^{r}\{1^{r}\}$$

$$= \{1\}^{\nu} + 2\sum_{0}^{\nu-1} (-1)^{\nu-r}\{1^{r}\} \qquad (3.40)$$

$$\Delta_{\frac{1}{2}}\Delta''_{\frac{1}{2}} = \Pi(2\cos\tfrac{1}{2}\phi_{r})\Pi(2i\sin\tfrac{1}{2}\phi_{r})$$

$$= \Pi 2i\sin\phi_{r}$$

$$= \Delta_{1} \qquad (3.41)$$

now $\Delta_{1}\Delta_{\frac{1}{2}} = \Delta_{\frac{1}{2}}\Delta''_{\frac{1}{2}}\Delta_{\frac{1}{2}}$

$$= \Delta''_{\frac{1}{2}}[\{1^{\nu}\} + 2\sum_{0}^{\nu-1}\{1^{r}\}] \qquad (3.42)$$

and $\Delta_{1}\Delta''_{\frac{1}{2}} = \Delta_{\frac{1}{2}}[\{1^{\nu} + 2\sum_{0}^{\nu-1}(-1)^{\nu-r}\{1^{r}\}] \qquad (3.43)$

The evaluation of the square of the basic difference character is more difficult. The principle part of the product is $\{2^{\nu}\}$. I have that

$$[1^{\nu}]^{2} = \sum_{s,r=0}[2^{\nu-s-2r}\ 1^{r}] \qquad (3.44)$$

$$[1^{\nu-1},-1]^{2} = \Sigma[\lambda'] \qquad (3.45)$$

where $[\lambda'] = [\lambda_{1},\lambda_{2},\cdots,\lambda_{\nu-1},-\lambda_{\nu}]$

and $\Sigma[\lambda]$ is the series in eqn (3.44),

and $[1^{\nu}][1^{\nu-1},-1] = \Sigma[2^{\nu-s-2r-1},1^{2r}] \qquad (3.46)$

Using the defining equation of Δ_1 and expressing the above results in S-functions, I obtain

$$\Delta_1^{\ 2} = \sum_{s=0}^{v} \sum_{r=0}^{s/2} f_s (-1)^{v-s} \{2^{s-2r}, 1^{2r}\} \tag{3.47}$$

where $f_s = 4$ except $f_v = 1$, $f_{v-1} = 3$.

The results, summarized in Table IV allow the evaluation of all products of rotation group characters.

13. SELECTION RULES

Conjugates: It is well known[27] that the matrix element of an operator H between wavefunctions A and B vanishes if the triple Kronecker product of the representations, describing the symmetry under some group, and the operator and of the wavefunctions, does not contain the identity. However for the unitary groups and the even dimensional rotation groups the representations are not, in general, self-conjugate and it is necessary to be more precise.

If a ket $|A\rangle$ transforms according to a representation Γ_A, then the bra $\langle A|$ will transform according to the conjugate representation $\Gamma_A{}^*$. Thus the matrix element

$$\langle A|H|B\rangle \text{ is zero}$$

$$\text{unless} \quad \Gamma_A{}^* \times \Gamma_H \times \Gamma_B \supset 1 \tag{3.48}$$

The coefficient $C_{\lambda\mu\nu}$ defined by the Kronecker product:

$$(\lambda) \times (\mu) = \sum C_{\lambda\mu\nu} (\nu) \tag{3.49}$$

TABLE IV: Products of the basic spin and difference characters of Rotation Groups

$n = 2\nu+1$

$$(\Delta_{\frac{1}{2}})^2 = \sum_{r=o}^{\nu} \{1^r\}$$

$n = 2\nu$

$$(\Delta_{\frac{1}{2}})^2 = \{1^\nu\} + 2 \sum_{r=0}^{\nu-1} \{1^r\}$$

$$(\Delta''_{\frac{1}{2}})^2 = \{1^\nu\} + 2 \sum_{r=0}^{\nu-1} (-1)^{\nu-r}\{1^r\}$$

$$\Delta''_{\frac{1}{2}} \Delta_{\frac{1}{2}} = \Delta_1$$

$$\Delta_{\frac{1}{2}} \Delta_1 = \Delta''_{\frac{1}{2}} (\{1^\nu\} + 2 \sum_{r=0}^{\nu-1} \{1^r\})$$

$$\Delta''_{\frac{1}{2}} \Delta_1 = \Delta'_{\frac{1}{2}} (\{1^\nu\} + 2 \sum_{r=0}^{\nu-1} (-1)^{\nu-r}\{1^r\})$$

$$(\Delta_1)^2 = \sum_{s=0}^{\nu} \sum_{r=0}^{s/2} f_s(-1)^{\nu-s} \{2^{s-2r}\ 1^{2r}\}$$

$f_s = 4$ except $f_\nu = 1$, $f_{\nu-1} = 3$

has the following symmetry properties:

$$C_{\lambda\mu\nu} = C_{\mu\lambda\nu} = C_{\nu^*\mu\lambda^*} \tag{3.50}$$

Since $C_{1\lambda\lambda} = 1$, $C_{1\lambda\mu} = 0 \quad \mu \neq \lambda$

we may rewrite eqn (3.48) as

$$\Gamma_B \times \Gamma_H \supset \Gamma_A \tag{3.48a}$$

$$\text{or} \qquad \Gamma_A{}^* \times \Gamma_B \supset \Gamma_H{}^* \tag{3.48b}$$

<u>Symmetrized Products:</u> Additional selection rules occur if in the matrix element $\langle A|H|B\rangle$ has the function and the operator symmetrized with respect to both a group and one of its subgroups; $|A\rangle \approx \Gamma_A\gamma_A$. If a pair of representations are equal, e.g. $\Gamma_B = \Gamma_H$, $\gamma_B = \gamma_H$, then the third representations must occur so that either both are in the symmetric or both in the antisymmetric parts of the squares.

For this example, the matrix element will be zero unless either $\Gamma_B \otimes \{2\} \supset \Gamma_A$ and $\gamma_B \otimes \{2\} \supset \gamma_A$ (3.49a)

or $\Gamma_B \otimes \{11\} \supset \Gamma_A$ and $\gamma_B \otimes \{2\} \supset \gamma_A$ (3.49b)

We emphasize that $\langle A|$ transforms as $\Gamma_A^*\gamma_A^*$.

14. RESOLUTION OF THE KRONECKER SQUARE

In a number of applications in physics the results of the above section are useful. It is clear[29,30] that the methods of plethysm provide a systematic answer to resolving the Kronecker square of any representation of any group. For the continuous groups, the outer products of S-functions correspond to the Kronecker product and thus outer plethysm is used to resolve the square. For point groups, being subgroups of the symmetric group, inner plethysm is required. I shall not investage such groups, but shall complete the analysis of the resolution of the square of all representations of rotation groups.

Littlewood derives from first principles, the resolution of the square of basic spin characters of the orthogonal groups into the symmetric and the antisymmetric parts. These are given in Table V. For the even dimensional rotation groups I write:

$$\Delta^{+}_{\frac{1}{2}} = [(\tfrac{1}{2})^{\nu}]; \qquad \Delta^{-}_{\frac{1}{2}} = [(\tfrac{1}{2})^{\nu-1},-\tfrac{1}{2}]$$

$$\Delta_{\frac{1}{2}} = \Delta^{+}_{\frac{1}{2}} + \Delta^{-}_{\frac{1}{2}}; \qquad \Delta''_{\frac{1}{2}} = \Delta^{+}_{\frac{1}{2}} - \Delta^{-}_{\frac{1}{4}} \qquad (3.50)$$

$$\therefore \quad \Delta_{\frac{1}{2}} + \Delta''_{\frac{1}{2}} = \Delta^{+}_{\frac{1}{2}} + \Delta^{+}_{\frac{1}{2}} \qquad (4.51a)$$

and

$$\Delta_{\frac{1}{2}} - \Delta''_{\frac{1}{2}} = \Delta^{-}_{\frac{1}{2}} + \Delta^{-}_{\frac{1}{4}} \qquad (4.51b)$$

TABLE V: Resolution of the Squares of Basic True and Spin Characters of Rotation Groups

n = 2ν+1

$$\Delta_{\frac{1}{2}} \otimes \{2\} = \{1^{\nu}\} + \{1^{\nu-3}\} + \{1^{\nu-4}\} + \{1^{\nu-7}\} + \{1^{\nu-8}\} + \cdots$$

$$\Delta_{\frac{1}{2}} \otimes \{11\} = \{1^{\nu-1}\} + \{1^{\nu-2}\} + \{1^{\nu-5}\} + \{1^{\nu-6}\} + \{1^{\nu-9}\} + \cdots$$

n = 2ν

$$\Delta_{\frac{1}{2}} \otimes \{2\} = \{1^{\nu}\} + \{1^{\nu-1}\} + \{1^{\nu-3}\} + 2\{1^{\nu-4}\} + \{1^{\nu-5}\} + \{1^{\nu-7}\} + 2\{1^{\nu-8}\} + \cdots$$

$$\Delta_{\frac{1}{2}} \otimes \{11\} = \{1^{\nu-1}\} + 2\{1^{\nu-2}\} + \{1^{\nu-3}\} + \{1^{\nu-5}\} + 2\{1^{\nu-6}\} + \{1^{\nu-7}\} + \cdots$$

$$\Delta''_{\frac{1}{2}} \otimes \{2\} = \tfrac{1}{2}(\Delta''_{\frac{1}{2}})^2 + \tfrac{1}{2}\Delta_1$$

$$= \tfrac{1}{2}\Delta_1 + \tfrac{1}{2}\{1^{\nu}\} - \{1^{\nu-1}\} + \{1^{\nu-2}\} - \{1^{\nu-3}\} + \cdots$$

$$\Delta''_{\frac{1}{2}} \otimes \{11\} = \tfrac{1}{2}(\Delta''_{\frac{1}{2}})^2 - \tfrac{1}{2}\Delta_1$$

$$= -\tfrac{1}{2}\Delta_1 + \tfrac{1}{2}\{1^{\nu}\} - \{1^{\nu-1}\} + \{1^{\nu-2}\} - \{1^{\nu-3}\} + \cdots$$

$$\Delta_1 \otimes \{2\} = \tfrac{1}{2}\Delta_1^{\,2} + \tfrac{1}{2}\Delta_1 \sum_{r=0} (-1)^r \{1^{\nu-2r}\}$$

TABLE V (contd)

$$\Delta_1 \otimes \{11\} = \tfrac{1}{2}\Delta_1{}^2 - \tfrac{1}{2}\Delta_1 \sum_{r=0} (-1)^r \{1^{\nu-2r}\}$$

Taking the symmetric part of the squares

$$\Delta_{\frac{1}{2}} \otimes \{2\} + \Delta''_{\frac{1}{2}}\otimes\{2\} - \Delta''_{\frac{1}{2}}\Delta_{\frac{1}{2}} \quad = \quad 2\Delta^{+}_{\frac{1}{2}} \otimes \{2\} + (\Delta^{+}_{\frac{1}{2}})^{2} \quad \text{etc.} \qquad (3.52)$$

By substituting in the known functions we get a series of relations of the form $\Delta''_{\frac{1}{2}} \otimes \{\lambda\} = 2\Delta^{\pm}_{\frac{1}{2}} \otimes \{\mu\} + \cdots$. Restrictions on $\Delta^{\pm}_{\frac{1}{2}} \otimes \{2\}$ and $\Delta^{\pm\prime}_{\frac{1}{2}} \otimes \{11\}$ and dimensional requirements lead to:

$$\Delta''_{\frac{1}{2}} \otimes\{2\} \quad = \quad \tfrac{1}{2}(\{1^{\nu}\} + \Delta_{1}) - \{1^{\nu-1}\} + \{1^{\nu-2}\} - \{1^{\nu-3}\} + \cdots \qquad (3.53a)$$

and

$$\Delta''_{\frac{1}{2}} \otimes \{11\} \quad = \quad \tfrac{1}{2}(\{1^{\nu}\} - \Delta_{1}) - \{1^{\nu-1}\} + \{1^{\nu-2}\} - \{1^{\nu-3}\} + \cdots \qquad (3.53b)$$

The evaluation of $\Delta_{1} \otimes \{2\}$ and $\Delta_{1} \otimes \{11\}$ follows the same steps to give the results in Table V.

Thus we may calculate the resolution of any character of any group.

e.g. $\left[\frac{3}{2}\ \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}\right] \otimes \{2\}$ of R_8

$$2\left[\frac{3}{2}\ \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}\right] \quad = \quad \Delta_{\frac{1}{2}}(\{1\} - \{0\}) + \Delta''_{\frac{1}{2}}(\{1\} + \{0\})$$

$$\therefore \; (2\left[\frac{3}{2}\ \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}\right]) \otimes \{2\} \quad = \quad 2\left[\frac{3}{2}\ \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}\right] \otimes \{2\} + \left[\frac{3}{2}\ \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}\right]^{2}$$

$$= \quad \Delta_{\frac{1}{2}} \otimes \{2\}(\{1\}-\{0\}) \otimes \{2\}$$

$$+ \Delta_{\frac{1}{2}} \otimes \{11\}(\{1\}-\{0\}) \otimes \{11\} + \Delta''_{\frac{1}{2}} \otimes \{2\}(\{1\}+\{0\}) \otimes \{2\}$$

$$+ \Delta''_{\frac{1}{2}} \otimes\{11\}(\{1\}+\{0\}) \otimes \{11\} + \Delta_{\frac{1}{2}}\Delta''_{\frac{1}{2}}(\{1\}-\{0\})(\{1\}+\{0\})$$

where we use the distributative properties of the plethysm, eqs (1.30, 1.32). Each term is expanded to give

$$2\left[\frac{3}{2}\ \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}\right] \otimes \{2\} = \{3111\} + \{211\} + 3\{22\} + \{31\} - \{2\} - \{11\} + \{0\} + \Delta_1\{2\}$$

Hence:

$$\left[\frac{3}{2}\ \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}\right] \otimes \{2\} = [3111] + [2200] + [2110] + [2000] + [1111] + [111\text{-}1] + [0000]$$

Although we have written an outer plethysm sign here and have in fact performed this operation on the S-function expression for the character of the group, we are in fact symmetrizing an inner product of the group characters - we are remaining within the one group. Thus the dimension check is given by the inner plethysm result of eqn (1.47).

For the special case of symmetrizing the square I obtain

$$f([\lambda] \otimes \{2\}) = f[\lambda](f[\lambda] + 1)/2 \qquad (3.54a)$$

and

$$f([\lambda] \otimes \{11\}) = f[\lambda](f[\lambda] - 1)/2 \qquad (3.54b)$$

For the example above, the degree of each side is thus: 1596

15. PLETHYSMS FOR GL_2 AND R_3

Plethysms of characters on two basis variables are often of use in physics. Plethysms for GL_2 may be evaluated by restricting the results for the same plethysm on an unrestricted number of variables. In the absence of such a table we may generate the plethysm required by use of the recursive relation[13]:

$$\{m\} \otimes \{k\} = \{m-2\} \otimes \{k\} + \{m\} \otimes \{k-2\} + (\{m-1\} \otimes \{k-1\})(\{m+k-1\} - \{m+k-3\}). \tag{3.55}$$

The following polynomial expansion due to Littlewood[31], for the plethysm of an R_3 representation and an S-function into only one part, is more suited to machine calculations

$$[n] \otimes \{p\} = \Sigma K_r [r]$$

where K_r is the coefficient of ρ^{-r} in the expansion of

$$\rho^{-np}(1-\rho) \prod_{i=1}^{p} \frac{(1-\rho^{2n+i})}{(1-\rho^{i})} . \tag{3.56}$$

This expression holds also for spin representations. A similar expression for the plethysm of a GL_2 representation allows us to make the following isomorphism between GL_2 and R_3

$$\{n\} \leftrightarrow [n/2]. \tag{3.57}$$

16. GENERAL BRANCHING RULES

The use of the algebra of plethysm allows us to calculate, directly and unambiguously, the branching rules between any compact group and a subgroup of lower dimension or a direct product of such groups[32]. Quite generally, given that the unary character [1] of the larger group decomposes to a sum of characters A under the restriction, then any character λ will decompose into the sum of characters given by $A \otimes \lambda$.

The branching rules for any group R_3 may therefore be easily calculated after defining our unary decomposition.

For example, to calculate the branching of [210] of R_7 to R_3 we note that [100] of R_7 branches to a single F state, i.e. the representation [3] of R_3. Hence the decomposition of [210] is given by $[3] \otimes [210]$. We express [210] in terms of S-functions, and then these into sums and products of partitions into one part, giving:

$$[3] \otimes [210] = [3] \otimes (\{2\}\{1\} - \{3\} - \{1\}).$$

Using the result, e.g. (1.27, 1.28), that the plethysm is distributive on the right with respect to both addition and multiplication, by using equation (3.55) and by multiplying together the R_3 representations in the usual manner we obtain

$$[210] \to [1] + 2[2] + [3] + 2[4] + 2[5] + [6] + [7] + [8].$$

This method of performing the plethysm on the symmetric parts of the right hand side is not always the easiest method. When branching to R_3 it is often easier to make use of the relation[13]

$$\{p\} \otimes \{1^m\} = \{p+1-m\} \otimes \{m\}. \qquad (3.58)$$

by expanding the S-functions in terms of their antisymmetric parts.

The saving in labour for classifying the orbital states of maximum multiplicity is immense. For example, in the t shell we use representations of R_{29}. The unary decomposition is $[100 \cdots 0] \to [14] = \{28\}$. Thus the states of maximum multiplicity for the quarter filled shell labelled by $[1^{14}]$ are easily found to be just the terms in

$$\{28\} \otimes [1^{14}] = \{28\} \otimes \{1^{14}\} = \{15\} \otimes \{14\}.$$

This has been expanded using the computer and there are found to be 34,670 states of total angular momentum of 23, a result that is difficult to obtain by the usual methods of determinantal states.

17. BRANCHING RULES FOR SPIN REPRESENTATIONS UNDER $R_n \to R_3$

Armstrong and Judd[33] have recently shown that the spin representations of the rotation groups R_n play a fundamental role in the analysis of the structure of electron configurations. The branching rules for the decomposition of the spin characters of R_n into characters of R_3 are especially important in their treatment.

The representations of R_3 depend on a single parametric angle θ and the character associated with the representation $D^{[J]}$ is

$$[J] = \sum_{\rho=0}^{2J} e^{i(J-\rho)\theta}, \tag{3.59}$$

where J may be integral of half-integral and ρ runs through positive integers. The representations of $R_{2\nu}$ and $R_{2\nu+1}$ each involve ν parametric angles θ_ε and in particular the character [1] for the vector representation $\Gamma^{[1]}$ of $R_{2\nu}$ is of the form

$$[1] = \sum_{\varepsilon=1}^{\nu} e^{\pm i\theta_\varepsilon}, \tag{3.60a}$$

while for $R_{2\nu+1}$ the corresponding character is

$$[1] = \sum_{\varepsilon=1}^{\nu} e^{\pm i\theta_\varepsilon} + 1. \tag{3.60b}$$

Under the restriction $R_n \to R_3$ the ν parametric angles become related and it is then possible to express the results of Eqs (3.60) in terms of a single parametric angle θ. If under $R_n \to R_3$ we have

$$[1] \to \Sigma g_J [J]$$

$$= \Sigma g_J \sum_{\rho=0}^{2J} e^{i(J-\rho)\theta} \tag{3.61}$$

then comparison of these equations allows the relationships between the ν parametric angles to be fixed immediately.

For example, if under $R_{2\ell+1} \to R_3$ we have $[1] \to [\ell]$ then comparison of Eq.(3.60) with Eq.(3.61) shows that the required relationship is

$$\theta_\varepsilon = \varepsilon\theta. \tag{3.62a}$$

Thus if under $R_9 \to R_3$ we have $[1] \to [4]$ then we must take

$$\theta_1 = \theta; \quad \theta_2 = 2\theta; \quad \theta_3 = 3\theta; \quad \theta_4 = 4\theta. \tag{3.26b}$$

If, however, under $R_9 \to R_3$ we have $[1] \to [0] + [1] + [2]$ then comparison of Eq.(3.59) with Eq.(3.60) leads to the choice

$$\theta_1 = 2\theta; \ \theta_2 = \theta_3 = \theta; \ \theta_4 = 0 \tag{3.63}$$

Likewise, if under $R_6 \to R_3$ we have $[1] \to [0] + [2]$ then comparison of Eq. (3.60) with Eq. (3.61) gives the relations

$$\theta_1 = 2\theta; \ \theta_2 = \theta; \ \theta_3 = 0. \tag{3.64}$$

Having defined the decomposition of the vector representations under the restriction $R_n \to R_3$, as in eqn (3.61) we may immediately find the corresponding decomposition for any other true representation λ of R_n by evaluating the terms in the plethysm

$$(\Sigma g_J[J]) \otimes [\lambda]. \tag{3.65}$$

The character associated with the basic spin character Δ of $R_{2\nu+1}$ may be expressed in terms of ν parametric angles θ_ε to give

$$\Delta = \Sigma e^{\frac{i}{2}(\pm\theta_1 \pm\theta_2 \pm \cdots \pm\theta_\nu)} \tag{3.66}$$

where the summation is over all possible combinations of the plus and minus signs. In the case of the even-dimensional rotation group $R_{2\nu}$ we have

$$\Delta_1 = e^{\frac{i}{2}(\pm\theta_1 \pm\theta_2 \pm \cdots \pm\theta_\nu)} \tag{3.67}$$

where the summation is over all combinations of signs involving an <u>even</u> number of minus signs. The conjugate spin character Δ_2 is of the same form except that the summation is over all possible combinations of signs involving an <u>odd</u> number of minus signs.

If the decomposition of the character of the vector representation $\Gamma^{[1]}$ of $R_{2\nu}$ or $R_{2\nu+1}$ under the restriction

$R_n \rightarrow R_3$ is defined then the relationships among the ν parametric angles is fixed and may be used in eqs (3.66) and (3.67) as the case may be. Comparison with eqn (3.59) leads immediately to the decomposition rule for the spin character.

Thus if under $R_9 \rightarrow R_3$ we have $[1] \rightarrow [4]$ the relationships between the four parametric angles are fixed by eqn (3.62b) which when employed in Eq. (3.66) and the result compared with eqn (3.59), leads immediately to the result

$$\Delta \rightarrow [2] + [5] \tag{3.68}$$

which may be verified as dimensionally correct. If, however, under $R_9 \rightarrow R_3$ we have $[1] \rightarrow [0] + [1] + [2]$ then we must use the parametric angle relationships of eqn (3.63) giving

$$\Delta \rightarrow 2[1] + 2[2]. \tag{3.69}$$

Likewise, if under $R_6 \rightarrow R_3$ we have $[1] \rightarrow [0] + [2]$ then use of Eq. (3.64) in Eq. (3.67) gives the result

$$\Delta_1 \rightarrow [3/2]. \tag{3.70}$$

The corresponding result for Δ_2 is identical to that for Δ_1. Comparison of Eqs (3.66) and (3.67) with Eqs (3.60) leads immediately to the result that if under $R_{2\ell+1} \rightarrow R_3$ we have $[1] \rightarrow [\ell]$ and $\Delta \rightarrow \Sigma g_L[L]$ while under $R_{2\ell+2} \rightarrow R_3$ we have $[1] \rightarrow [0] + [\ell]$ then also $\Delta_1 \rightarrow \Sigma g_L[L]$.

18. CANONICAL CHAINS

Recently Gilmore[34] rederived the expression[35] for the canonical chain for characters, true and spin, of the rotation group. It is proposed to give a more elegant derivation in terms of the algebra of S-functions.

The canonical chain is

$$R_n \to R_{n-1} \to R_{n-2} \cdots \to R_2 \tag{3.71}$$

The basic branching rule for each step is

$$[1]' \to [0] + [1] \tag{3.72}$$

therefore, as for all branching rules,

$$[\lambda]' \to ([0] + [1]) \otimes [\lambda]' \tag{3.73}$$

For true representations

$$[\lambda]' = \{\lambda\}'/(-1)^{\frac{1}{2}p}\{\gamma\}' = \Sigma\{\mu\}' \tag{3.74}$$

$$\therefore [\lambda]' \to (\{0\} + \{1\}) \otimes (\Sigma\{\mu\})$$

$$= \Sigma(\{0\} \otimes \{\xi\})(\{1\} \otimes (\{\mu\}/\{\xi\}))$$

but $\{0\} \otimes \{\xi\} = 0$ unless $\{\xi\} = \{h\}$

$$\therefore [\lambda]' \to \{1\} \otimes (\{\mu\}/\{h\})$$

$$= \{\mu\}/\{h\}$$

$$= [\{\mu\}/\{h\}/\{\delta\}]'$$

where $[\{\nu\}]'$ means take the resultant series as orthogonal group characters

$$= [\{\lambda\}/(-1)^{\frac{1}{2}p}\{\gamma\}/\{h\}/\{\delta\}]'$$

$$= [\{\lambda\}/(-1)^{\frac{1}{2}p}\{\gamma\}.\{h\}.\{\delta\})]'$$

Thus $[\lambda]' = [\{\lambda\}/\{h\}]'$ since $(-1)^{\frac{1}{2}p}\{\gamma\}\{\delta\} = \{0\}$ (3.75)

For the step $R_{2\nu+1} \rightarrow R_{2\nu}$ no modification rules are required except that for characters into ν parts when we have $O_{2\nu} \rightarrow R_{2\nu}$.

$$[\mu]' \rightarrow [\mu] + [\mu'].$$

For the step $R_{2\nu} \rightarrow R_{2\nu-1}$ no modification rules are necessary except again for the characters of ν parts, difference characters occur in equation (3.74), namely

$$[\lambda] = \tfrac{1}{2}(\{\lambda\}/(-1)^{\frac{1}{2}p}\{\gamma\} \pm \Delta_1\{\lambda'\}/(-1)^{\frac{1}{2}p}\{\alpha\}) \qquad (3.74a)$$

where $\{\lambda'\} = \{\lambda_1-1,\lambda_2-1,\cdots,|\lambda_\nu|-1\}$.

In the plethysm we have $A \otimes \Delta_1 \equiv 0$ and therefore

$$[\lambda_1,\lambda_2,\cdots,\pm\lambda_\nu] \rightarrow \tfrac{1}{2}[\{\lambda\}/\{h\}] \qquad (3.75a)$$

where we use modification rules as required.

e.g. $R_6 \rightarrow R_5$ for $[21\pm1]$ we have:

$$[21\pm1] \rightarrow \tfrac{1}{2}[\{\lambda\}/\{h\}] = \tfrac{1}{2}([211] + [21] + [111] + [11])$$

$$\rightarrow [21] + [11]$$

where we used either Murnaghan's modification rules[13], or expressed the characters in terms of S-functions on the five variables, reduced the number of parts, and branched back down to R_5.

For spin representations we follow the same derivation, except $[\lambda+\frac{1}{2}] = \Delta_{\frac{1}{2}}\{\lambda\}/(-1)^{\frac{1}{2}(p+r)}\{\varepsilon\}$ and we use the corresponding inverse relation - leading to the same result.

CHAPTER 4

GENERALIZED RACAH TENSORS AND THE STRUCTURE OF MIXED CONFIGURATIONS

1. INTRODUCTION

For a set of wavefunctions $\psi_1, \psi_2, \cdots, \psi_n$ we may define a vector representation $\Phi = (\phi_i)$, where ϕ_i is the coefficient of ψ_i in Φ. Linear transformations among the functions

$$\psi_i' = \alpha_{ij} \psi_j$$

may be represented by a matrix $A = (\alpha_{ij})$ so that:

$$\Phi' = A\Phi$$

From the normalization condition of these complex wave functions, we find that the transformation matrix A is unitary. It can also be produced by infinitesimal transformations. In fact any such transformation can be produced a limited number of such transformations. These "generators" are an arbitrarily chosen maximal set of linearly independent unitary matrices of the same order as A.

It is the purpose of the present chapter to investigate the group theoretical properties of the various generators that may be chosen to produce the transformations between the wave-functions of configurations of electrons or nucleons. Much of the previous work has been restricted to the LS coupled states of configurations of electrons of a given field orbital quantum number ℓ. Feneuille[36] studied a system whereby we have two such shells mixing - $(s+p)^N$ and recently Morrison[37] studied two j-j coupled shells. Nuclear physicists have studied similar systems[38].

In this chapter we shall attempt to give the grou structure of all such mixed configurations. A choice of generators of a possible subgroup - R_4 - is made so that this group's labels may be used for the case when R_4 is the symmetry of the physical system (e.g. the hydrogen atom). The generators are chosen, after the manner of Racah, to always have well defined transformation properties under R_3 and we shall call them generalized Racah tensors, or simply Racah tensors.

2. GENERALIZED TENSOR OPERATORS

Following Elliott[38] and Feneuille[36] let us define the tensor operators $\underset{\sim}{v}^{(k)}(A,B)$ and $\underset{\sim}{w}^{(\kappa k)}(A,B)$ in terms of their reduced matrix elements between single particle wave functions:

$$\langle C||\underset{\sim}{v}^{(k)}(A,B)||D\rangle = \delta(A,C)\delta(B,D)[k]^{\frac{1}{2}} \qquad (4.1a)$$

$$\langle sC \| w^{(\kappa k)}(A,B) \| sD\rangle = \delta(A,C)\delta(B,D)[\kappa,k]^{\frac{1}{2}} \qquad (4.1b)$$

with the usual notation $[x,y,\cdots,z] \equiv (2x+1)(2y+1)\cdots\ (2z+1)$. We use capital latin letters to indicate arbitrary values of the single particle angular momentum.

A component $w^{(\kappa k)}_{\pi q}(A,B)$ operating on a single electron wave function gives:

$$w^{(\kappa k)}_{\pi q}(A,B)|s\ell m_s m_\ell\rangle = \sum_{\ell',m'_\ell,m'_s} \delta(A,\ell')\delta(B,\ell)(-1)^{\ell'+s-m'_\ell-m'_s}$$

$$\times [\kappa,k]^{\frac{1}{2}} \begin{pmatrix} s & \kappa & s \\ -m'_s & \pi & m_s \end{pmatrix} \begin{pmatrix} \ell' & k & \ell \\ -m'_\ell & q & m_\ell \end{pmatrix} |s\ell' m'_s m'_\ell\rangle\ , \qquad (4.2)$$

from which we may deduce the general commutator expression,

$$[w^{(\kappa_1\ k_1)}_{\pi_1\ q_1}(A,B), w^{(\kappa_2\ k_2)}_{\pi_2\ q_2}(C,D)]$$

$$= \sum_{\kappa_3,k_3,\pi_3,q_3} (-1)^{2s+\kappa_3+k_3-\pi_3-q_3}$$

$$\times [\kappa_1,\kappa_2,\kappa_3,k_1,k_2,k_3]^{\frac{1}{2}} \begin{pmatrix} \kappa_1 & \kappa_2 & \kappa_3 \\ \pi_1 & \pi_2 & -\pi_3 \end{pmatrix} \begin{pmatrix} k_1 & k_2 & k_3 \\ q_1 & q_2 & -q_3 \end{pmatrix} \begin{Bmatrix} \kappa_1 & \kappa_2 & \kappa_3 \\ s & s & s \end{Bmatrix}$$

$$\times [\delta(B,C)(-1)^{A+D+\kappa_1+\kappa_2+k_1+k_2} \begin{Bmatrix} k_1 & k_2 & k_3 \\ D & A & B \end{Bmatrix} w^{(\kappa_3\ k_3)}_{\pi_3\ q_3}(A,D)$$

$$- \delta(A,D)(-1)^{B+C+\kappa_3+k_3} \begin{Bmatrix} k_1 & k_2 & k_3 \\ C & B & A \end{Bmatrix} w^{(\kappa_3 k_3)}_{\pi_3 q_3}(C,B)]. \qquad (4.3)$$

I define the linear combinations

$$\overset{\pm}{\underset{\sim}{w}}{}^{(\kappa k)}(A,B) = \underset{\sim}{w}^{(\kappa k)}(A,B) \pm (-1)^{\kappa+k+A-B}\, \underset{\sim}{w}^{(\kappa k)}(B,A) \tag{4.4}$$

and obtain the commutators:

$$[\overset{+}{w}{}^{(\kappa_1 k_1)}_{\pi_1 q_1}(A,B), \overset{\pm}{w}{}^{(\kappa_2 k_2)}_{\pi_2 q_2}(C,D)] = \sum_{\kappa k \pi q} (-1)^{\kappa-\pi+k-q+A+D+2s}$$

$$\times [\kappa_1,\kappa_2,\kappa,k_1,k_2,k]^{\frac{1}{2}} \begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix} \begin{pmatrix} \kappa_1 & \kappa_2 & \kappa \\ \pi_1 & \pi_2 & -\pi \end{pmatrix} \begin{Bmatrix} \kappa_1 & \kappa_2 & \kappa \\ s & s & s \end{Bmatrix}$$

$$\times \Bigg\{ \delta(B,C)(-1)^{k_1+k_2+\kappa_1+\kappa_2} \begin{Bmatrix} k_1 & k_2 & k \\ D & A & B \end{Bmatrix} \overset{\mp}{w}{}^{(\kappa k)}_{\pi q}(A,D)$$

$$\pm\ \delta(A,D) \begin{Bmatrix} k_1 & k_2 & k \\ C & B & A \end{Bmatrix} \overset{\mp}{w}{}^{(\kappa k)}_{\pi q}(B,C)$$

$$\pm\ \delta(B,D)(-1)^{\kappa_1+k_1} \begin{Bmatrix} k_1 & k_2 & k \\ C & A & B \end{Bmatrix} \overset{\mp}{w}{}^{(\kappa k)}_{\pi q}(A,C)$$

$$+\ (A,C) \begin{Bmatrix} k_1 & k_2 & k \\ C & B & A \end{Bmatrix} \overset{\mp}{w}{}^{(\kappa k)}_{\pi q}(B,D) \Bigg\} \tag{4.5a}$$

and

$$[\overset{-}{w}{}^{(\kappa_1 k_1)}_{\pi_1 q_1}(A,B), \overset{\pm}{w}{}^{(\kappa_2 k_2)}_{\pi_2 q_2}(C,D)] = \sum_{\kappa k \pi q} (-1)^{\kappa-\pi+k-q+A+D+2s}$$

$$\times [\kappa_1,\kappa_2,\kappa,k_1,k_2,k]^{\frac{1}{2}} \begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix} \begin{pmatrix} \kappa_1 & \kappa_2 & \kappa \\ \pi_1 & \pi_2 & -\pi \end{pmatrix} \begin{Bmatrix} \kappa_1 & \kappa_2 & \kappa \\ s & s & s \end{Bmatrix}$$

$$\times \Bigg[\delta(B,C)(-1)^{k_1+k_2+\kappa_1+\kappa_2} \begin{Bmatrix} k_1 & k_2 & k \\ D & A & B \end{Bmatrix} \overset{\pm}{w}{}^{(\kappa k)}_{\pi q}(A,D)$$

$$\mp \delta(A,D) \begin{Bmatrix} k_1 & k_2 & k \\ C & B & A \end{Bmatrix} \overset{\pm}{w}{}^{(\kappa k)}_{\pi q}(B,C)$$

$$\pm \delta(B,D)(-1)^{\kappa_1+k_1} \begin{Bmatrix} k_1 & k_2 & k \\ C & A & B \end{Bmatrix} \overset{\pm}{w}{}^{(\kappa k)}_{\pi q}(A,C)$$

$$- \delta(A,C)(-1)^{\kappa_2+k_2} \begin{Bmatrix} k_1 & k_2 & k \\ D & B & A \end{Bmatrix} \overset{\pm}{w}{}^{(\kappa k)}_{\pi q}(B,D) \Bigg] \qquad (4.5b)$$

We note that the set $\overset{-}{\underset{\sim}{w}}{}^{(\kappa k)}(A,B)$ is closed under commutation but that the set $\overset{+}{\underset{\sim}{w}}{}^{(\kappa k)}(A,B)$ is in general not closed, in the sense that its commutators can produce terms of the form $\overset{-}{\underset{\sim}{w}}{}^{(\kappa k)}(A,B)$ etc. We could, of course, choose different sets, e.g. for two configurations the set $\overset{+}{\underset{\sim}{w}}{}^{(\kappa k)}(A,B)$ $(A \neq B)$ and $\underset{\sim}{w}^{(\kappa k)}(A,A)$, $\underset{\sim}{w}^{(\kappa k)}(B,B)$ $(\kappa+k)$ odd will be closed, but I hope to demonstrate shortly that the set of all $\overset{-}{\underset{\sim}{w}}{}^{(\kappa k)}(A,B)$ is the most suitable choice for all mixed configurations.

The choices

$$\bar{\underset{\sim}{w}}^{(\kappa k)}(A,B) = \underset{\sim}{w}^{(\kappa k)}(A,B) - (-1)^{\kappa+k}\,\underset{\sim}{w}^{(\kappa k)}(B,A) \qquad (4.6a)$$

$$\bar{\underset{\sim}{w}}^{(\kappa k)}(A,B) = \underset{\sim}{w}^{(\kappa k)}(A,B) - (-1)^{A+B+\kappa+k}\,\underset{\sim}{w}^{(\kappa k)}(B,A) \qquad (4.6b)$$

$$\overset{+}{\underset{\sim}{w}}{}^{(\kappa k)}(A,B) = \underset{\sim}{w}^{(\kappa k)}(A,B) + \underset{\sim}{w}^{(\kappa k)}(B,A) \qquad (4.6c)$$

have been taken by Feneuille[36], Morrison[37] and Elliott[38] respectively. Alper and Sinanoglu[39] have also used (4.6c) in their recent work on R_4. The above choices all have their disadvantages. It will be shown in the next section that Eq. (4.6a) does not contain the generators of the group R_4 but is equivalent to that of Eq. (4.4) where orbitals of the same parity are involved (e.g. $(s+d)^N$). The choice of Eq. (4.6b) is equivalent to that of Eq. (4.4) for integral A and B but does not reduce to Judd's operators[27] for half-integral values of A and B. The linear combination given in Eq. (4.6c) must be rejected as it fails to close under commutation.

The linear combinations defined by Eq. (4.4) satisfy the closure requirements in all cases and yield the appropriate generators for R_4 as a subgroup and reduce to the special cases studied by Judd[27], Feneuille[36] and Morrison[37].

Later we shall have occasion to use both the operators $\underset{\sim}{w}_i^{(\kappa k)}(A,B)$ and $\underset{\sim}{W}^{(\kappa k)}(A,B) \equiv \sum_i \underset{\sim}{w}_i^{(\kappa k)}(A,B)$ where $\underset{\sim}{w}_i^{(\kappa k)}(A,B)$ is the operator that acts only between states of the i-th electron and $\underset{\sim}{W}^{(\kappa k)}(A,B)$ acts between states of all electrons. Both sets of operators satisfy the commutation relations of Eqs (4.3) and (4.5). It is easily shown that

$$\underset{\sim}{w}^{(ok)}(A,B) \equiv \frac{1}{\sqrt{2}} v^{(k)}(A,B)$$

and all the commutation relations given in terms of $\underset{\sim}{w}^{(ok)}(A,B)$ may be reduced to those for $\underset{\sim}{v}^{(k)}(A,B)$ by omitting the quantum numbers dependent on spin.

3. INFINITESIMAL OPERATORS FOR R_4

We now wish to use the properties of the $v^{(k)}(A,B)$ tensor operators to construct a set of infinitesimal operators for the four dimensional rotation group R_4 which leave invariant the quadratic form $x_1^2+x_2^2+x_3^2+x_4^2$. The Lie algebra for R_4 may be defined in terms of six infinitesimal operators[40]

$$J_{\lambda\mu} = i(x_\mu \frac{\partial}{\partial x_\lambda} - x_\lambda \frac{\partial}{\partial x_\mu}) \quad (\lambda,\mu = 1,2,3,4) \qquad (4.7)$$

Putting $J_0 = J_{23}$, $J_{\pm 1} = \pm\sqrt{2}\,(J_{31} \pm iJ_{12})$

$$N_0 = J_{41}, \quad N_{\pm 1} = \pm\sqrt{2}\,(J_{42} \pm iJ_{43})$$

leads to the set of commutation relations

$$[J_i, J_j] = -\varepsilon_{ijk} J_k = [N_i, N_j]$$
$$[J_i, N_j] = -\varepsilon_{ijk} N_k \qquad (4.8)$$

I shall now obtain two sets of operators which satisfy these commutation relations and at the same time fix the phases of our $\bar{\underset{\sim}{v}}^{(k)}(A,B)$ operators.

It is well-known that not only $\underset{\sim}{L} = \frac{1}{h}\, r \times p$ but also the Runge-Lenz vector[41]

$$\underset{\sim}{A} = \left[\frac{z^2 e^4 m}{-2h^2 E}\right]^{\frac{1}{2}} \frac{1}{2Ze^2mh}(\underset{\sim}{L} \times \underset{\sim}{p} - \underset{\sim}{p} \times \underset{\sim}{L}) + \frac{\underset{\sim}{r}}{r} \,. \qquad (4.9)$$

commute with the hydrogenic Hamiltonian. The matrix elements of $\underset{\sim}{A}$ between single electron states may be calculated following Biedenharn[42] or from first principles to give

$$\langle n\ell m|A_z|n\ell' m'\rangle = \langle n\ell' m'|A_z|n\ell m\rangle$$
$$= \left[\frac{(n-\ell-1)(n+\ell+1)(\ell+m+1)(\ell-m+1)}{(2\ell+1)(2\ell+3)}\right]^{\frac{1}{2}} . \qquad (4.10)$$

Using this result we may readily show that

$$\underset{\sim}{A} = \sum_{\ell=0}^{n-2} [(n-\ell-1)(n+\ell+1)(\ell+1)/3]^{\frac{1}{2}} \{\underset{\sim}{V}^{(1)}(\ell,\ell+1) - \underset{\sim}{V}^{(1)}(\ell+1,\ell)\} . \qquad (4.11)$$

This, taken with the known result[50]

$$\underset{\sim}{L} = \sum_{\ell=0}^{n-1} [\ell(\ell+1)(2\ell+1)/3]^{\frac{1}{2}} \underset{\sim}{V}^{(1)}(\ell,\ell) \qquad (4.12)$$

gives us a set of six operators that satisfy the commutation relations of Eq. (4.8). The phase choice for $\underset{\sim}{A}$ means that $\underset{\sim}{A}$ is a simple linear combination of the $\bar{\underset{\sim}{V}}^{(1)}(\ell,\ell')$ operators defined in Eq. (4.4). Other choices of phases make it impossible to form an operator A out of the operators of the larger rotation group formed by the set of all $\bar{V}^{(k)}(\ell,\ell')$ operators. We must now take up the study of these larger groups.

4. CONSTRUCTION OF ROOT FIGURES USING $\underset{\sim}{V}^{(k)}(A,B)$ AND $\underset{\sim}{W}^{(\kappa k)}(A,B)$ OPERATORS

In this section we largely follow the arguments of Chapters 5 and 6 of Judd's text[27] and construct root figures using general sets of the operators $\underset{\sim}{V}^{(k)}(A,B)$ and $\underset{\sim}{W}^{(\kappa k)}(A,B)$. These operators for A, B,$\cdots$,F = $\ell_1, \ell_2, \cdots, \ell_n$ form the infinitesimal operators of the groups U_X and U_{2X} respectively, where

$$X = \sum_{i=1}^{n} (2\ell_i+1)$$

and ℓ is integral or half-integral.

<u>The Orbital Unitary Group:</u> Let us first consider the case of the $\underset{\sim}{V}^{(k)}(A,B)$ type operators. Using the methods of

Jucys et al.[43] we may show that the linear combinations

$$\Gamma_{ab}(A,B) = \sum_{k,q} (-1)^{A-a}[k]^{\frac{1}{2}} \begin{pmatrix} A & k & B \\ -a & q & b \end{pmatrix} V^{(k)}_{q}(A,B) \qquad (4.13)$$

satisfy the commutation relations

$$[\Gamma_{ab}(A,B),\Gamma_{cd}(C,D)] = \delta(B,C)\delta(b,c)\Gamma_{ad}(A,D)$$

$$- \delta(A,D)\delta(a,d)\Gamma_{cb}(C,B) \qquad (4.14)$$

The self-commuting Weyl operators[44] $H_{I,i} = \Gamma_{ii}(I,I)$ have eigenvalues 0,±1 to give us the roots $\underset{\sim}{e}_{Aa}-\underset{\sim}{e}_{Bb}$ with $\Gamma_{ab}(A,B)$, these roots being appropriate to U_X.

<u>Orbital Subgroups:</u> The subgroups of U_X formed by the set of tensors $\underset{\sim}{\bar{v}}^{(k)}(A,B)$ set a somewhat more complicated problem. We define the linear combination

$$H_{ab}(A,B) = \sum_{k,q} k^{\frac{1}{2}}(-1)^{A-a} \begin{pmatrix} A & k & B \\ -a & q & b \end{pmatrix} \bar{V}^{(k)}_{q}(A,B) \qquad (4.15)$$

giving

$$H_{ab}(A,B) = (-1)^{A+B+a+b+1} H_{-b-a}(B,A)$$

which are therefore not all linearly independent for $A \equiv B$. Forming the commutator gives

$$
\begin{aligned}
H_{ab}(A,B),\ H_{cd}(C,D) &= \delta(B,C)\delta(b,c)\ H_{ad}(A,D) \\
&\quad - \delta(A,D)\delta(a,d)\ H_{cb}(C,B) \\
+ (-1)^{A+B+a+b+1}\{\delta(A,C)\delta(-a,c)\ H_{-bd}(B,D) & \\
&\quad - \delta(B,D)\delta(-b,d)\ H_{c-a}(C,A)\} \quad (4.16)
\end{aligned}
$$

It can easily be shown that the operators $H_{I,i} = H_{ii}(I,I)$ with $i > 0$ acting on the remaining operators $H_{ab}(A,B)$, with $a \neq 0 \neq b$ yield all the roots $\pm \underset{\sim}{e}_{Aa} \pm \underset{\sim}{e}_{Bb}$.

a) Half integral ℓ: For the case where the angular momentum set, A, B,··· is half-integral the set of roots includes the roots $\pm 2\underset{\sim}{e}_{Aa}$ coming from

$$H_{a-a}(A,A) = (-1)^{2A+1} H_{-aa}(A,A) \quad \text{for } a \neq 0$$

The complete set of roots then gives the customary root figure for the symplectic group Sp_X where X is an even integer.

b) Integral ℓ: In the case of the rotation group R_X the roots $\pm 2\underset{\sim}{e}_{Aa}$ do not occur since $(-1)^{2A+1} = -1$. However, there remain operators of the form $H_{ao}(A,B)$ with $a \neq 0$ and $H_{oo}(A,B) = -H_{oo}(BA)$ (hence $A \neq B$). We must complement the above Weyl operators $H_{I,i}$ with a set $H_{IJ} = (-1)^{(A+B+1)/2}$ $H_{oo}(A,B)$, $(-1)^{(C+D+1)/2} H_{oo}(C,D)$, etc, which satisfy $H_{IJ} = H_{JI}$. (It will be noted that we must have this phase choice which often leads to imaginary operators but real roots. The simplest case for which this occurs is for $(s+d)^n$ when the characters of R_6 are complex.) The operators $H_{co}(C,A) \pm (-1)^{(A+B+1)/2} H_{co}(C,B)$ with $c \neq 0$ give the roots $\pm \underset{\sim}{e}_{AB} \pm \underset{\sim}{e}_{Cc}$. For every set of four angular momenta A,B,C,D etc considered we must also have the combinations

$$H_{oo}(C,A) \pm (-1)^{(A+B+1)/2} H_{oo}(C,B)$$

$$+ (-1)^{(C+D+1)/2}\left(H_{oo}(D,A) \pm (-1)^{(A+B+1)/2} H_{oo}(D,B)\right)$$

and

$$H_{oo}(C,A) \pm (-1)^{(A+B+1)/2} H_{oo}(C,B) - (-1)^{(C+D+1)/2}$$

$$\left(H_{oo}(D,A) \pm (-1)^{(A+B+1)/2} H_{oo}(D,B)\right)$$

which give the roots $\pm \underset{\sim}{e}_{AB} \pm \underset{\sim}{e}_{CD}$. This completes the root figure for the even dimensional rotation groups. In the case of an odd number of angular momenta we have finally the operators $H_{AO}(A,L)$ and $H_{oo}(L,A) \pm (-1)^{(A+B+1)/2}$ $H_{oo}(L,B)$ giving the roots $\pm \underset{\sim}{e}_{Aa}$ and $\pm \underset{\sim}{e}_{AB}$ required for the root figure of the odd dimensional rotation group.

<u>The Group Sp_{2X}:</u> For integral A,B,... and half-integral spin the tensors $\bar{\underset{\sim}{W}}^{(\kappa k)}(A,B)$ generate the symplectic group in 2X dimensions. This group gives rise to the so-called seniority classification scheme first used by Racah[2].

Let us now consider the $\bar{\underset{\sim}{W}}^{(\kappa k)}(A,B)$ operators. In a similar fashion to the above we define the operators

$$H_{\alpha\beta ab}(AB) = \sum_{\kappa k\pi q} (-1)^{s-m_s A a-a}[\kappa,k]^{\frac{1}{2}} \begin{pmatrix} s & \kappa & s \\ -\alpha & \pi & \beta \end{pmatrix} \begin{pmatrix} A & k & B \\ -a & p & b \end{pmatrix}$$

$$\bar{W}^{(\kappa k)}_{\pi q}(A,B) \qquad (4.17)$$

These lead to the establishment of the root figure for Sp_{2X}. Several choices exist for the phases of the Weyl H operators. We shall choose

$$H_{Aa} = H_{\frac{1}{2}\frac{1}{2}aa}(A,A) \qquad -A \leqslant a \leqslant A.$$

This choice is made so that

$$\sum_{A,a} H_{Aa} = \sqrt{2} \sum_{A} [A]^{\frac{1}{2}} W^{(10)}_{00}(A,A) = 2S_Z$$

and thus ensuring that the function of highest weight belonging to a representation of Sp_{2X} will have the highest possible spin.

<u>The Unitary Group U_{2X}:</u> The complete set of operators $\underset{\sim}{W}^{(\kappa k)}(A,B)$ form a group, U_{2X}, and the construction root figure follows simply the method of the orbital unitary group U_X except we are required to sum over both the spin and orbital quantum numbers.

5. CASIMIR'S OPERATORS AND EIGENVALUES

The structure constants $c_{\sigma\rho}^{\ \ \tau}$ of a group are defined by the commutation properties of the infinitesimal operators, X_σ, viz.,

$$[X_\sigma, X_\rho] = \sum_\tau c_{\sigma\rho}^{\ \ \tau} X_\tau .$$

The metric tensor $g_{\sigma\lambda}$ is obtained in terms of the structure constants as[27]

$$g_{\sigma\lambda} = c_{\sigma\rho}^{\ \ \tau}\, c_{\tau\lambda}^{\ \ \rho} .$$

For semi-simple groups the metric tensor has its inverse $g^{\rho\lambda} = (g_{\sigma\lambda})^{-1}$ and the Casimir operator[45] G is defined as

$$G = g^{\rho\lambda} X_\rho X_\lambda .$$

From its construction it is evident that G commutes with all the operators of the group. Racah[2] has shown that the eigenvalues of the Casimir operator may be expressed in the form $\underset{\sim}{K}^2 - \underset{\sim}{R}^2$ where $\underset{\sim}{R} = \frac{1}{2}\Sigma\underset{\sim}{\alpha}^+$ and $K_i = R_i + w_i$ with $\underset{\sim}{\alpha}^+$ being a positive root and w_i the i-th component of the highest weight of the representation.

The eigenvalues λ_w of the Casimir operator $G(R_n)$ $(n = 2\nu$ or $2\nu+1)$ or of $G(Sp_n)$ $(n = 2\nu)$ may be found by acting the Casimir operator on the eigenket $|W\rangle \equiv |w_1 \cdots w_\nu\rangle$ which forms a basis for the representation $[w_1 \cdots w_\nu]$ of R_n or $\langle w_1 \cdots w_\nu\rangle$ of Sp_n to yield

$$\text{for } R_n \qquad \lambda_w = \frac{1}{2(n-2)} \sum_{i=1}^{\nu} w_i(w_i+n-2i) \tag{4.18}$$

$$\text{and for } Sp_n \qquad \lambda_w = \frac{1}{2(n-2)} \sum_{i=1}^{\nu} w_i(w_i+n-2i+2). \tag{4.19}$$

The Casimir operator may be conveniently expressed in terms of the operators defined in Eq. (4.15) for R_X as

$$2\,(X-2)G = \tfrac{1}{2} \sum_{A,B} \sum_{a,b} H_{ab}(A,B)\, H_{ba}(B,A) \tag{4.20}$$

$$= 2\sum_{A} \sum_{k\ \mathrm{odd}} (\underset{\sim}{V}^{(k)}(A,A))^2 + (-1)^{k+1} \sum_{A<B} \sum_{k} (\underset{\sim}{\bar{V}}^{(k)}(A,B))^2 \tag{4.21}$$

and for Sp_{2X} we use the operators of Eq. (4.17) to obtain

$$4(X-1)G(Sp_{2X}) = \tfrac{1}{2} \sum_{A,B} \sum_{a,b} \sum_{\alpha,\beta} H_{\alpha\beta ab}(A,B)\, H_{\beta\alpha ba}(B,A)$$

$$= 2 \sum_{A} \sum_{\kappa,k} (\underset{\sim}{W}^{(\kappa k)}(A,A))^2 + (-1)^{\kappa+k+1}$$

$$\sum_{A<B} \sum_{\kappa,k} (\underset{\sim}{\bar{W}}^{(\kappa k)}(A,B))^2 \tag{4.22}$$

where $\kappa+k$ is <u>odd</u> in the first summation.

The above results are useful for constructing eigenfunctions symmetrized with respect to the relevant representations of the transformation group used to classify the multiconfiguration states.

6. TRANSFORMATION PROPERTIES OF STATES AND OPERATORS

In this section I derive a correspondence between the transformation properties of the $\overset{\pm}{W}{}^{(\kappa k)}_{\pi q}(A,B)$ operators and the symmetric and antisymmetric combinations of two particle states.

Following Fano and Racah[46] we denote the vector coupled states of particle 1 in orbital A and particle 2 in orbital B, coupled to spin and orbital ranks κ and k with z-projections π and q respectively by $(12|AB\ \kappa k\pi q\rangle$. We then define the symmetric (+) and antisymmetric (-) combinations as

$$|AB\kappa k\pi q\rangle^{\pm} = [(12|AB\kappa k\pi q\rangle \pm (21|AB\kappa k\pi q\rangle] \tag{4.23}$$

Acting $\overset{-}{W}{}^{(\kappa_1 k_1)}_{\pi_1 q_1}(A,B)$ on a ket $|CD\kappa_2 k_2\pi_2 q_2\rangle^{\pm}$ gives a result equivalent to the commutator

$[\overset{-}{W}{}^{(\kappa_1 k_1)}_{\pi_1 q_1}(A,B),\ \overset{\mp}{W}{}^{(\kappa_2 k_2)}_{\pi_2 q_2}(C,D)]$ and thus proving

that the operators $\overset{\pm}{W}{}^{(\kappa k)}_{\pi q}(A,B)$ have the same symmetry transformation properties under the operations of Sp_{2X} and its subgroups as the two-particle states $|AB\kappa k\pi q\rangle^{\mp}$, i.e. the operators $\overset{+}{W}{}^{(\kappa k)}_{\pi q}(A,B)$ transform like fermions and the $\overset{-}{W}{}^{(\kappa k)}_{\pi q}(A,B)$ like bosons.

As the operators $\overset{+}{\underset{\sim}{W}}{}^{(\kappa k)}(A,B)$ transform the sets $\overset{+}{\underset{\sim}{W}}{}^{(\kappa k)}(A,B)$ and $\overset{-}{\underset{\sim}{W}}{}^{(\kappa k)}(A,B)$ into each other it is apparent that they must, together, span a single representation $\{\lambda\}$ of the unitary group U_{2X}. The operators connect states of the same number of particles and so we have

$$\{\lambda\}\{1^n\} \supset \{1^n\} \quad \text{for all } n$$

thus

$$\{1^n\}\{1^n\}^* \equiv \{1^n\}\{1^{2X-n}\} \supset \{\lambda\}$$

We find that the complete set of tensors $\underset{\sim}{W}^{(\kappa k)}(A,B)$ transform as the $\{21^{2X-2}0\}$ representation of U_{2X} with the exception of the scalar operator

$$\sum_A [A]^{\frac{1}{2}} W^{(00)}_{00}(A,A)$$

which transforms as $\{0\}$.

We have the branching rules for $U_{2X} \rightarrow Sp_{2X}$:

$$\{21^{2X-2}0\} \rightarrow \langle 2\rangle + \langle 11\rangle$$

$$\{0\} \rightarrow \langle 0\rangle. \tag{4.24}$$

Similar comments will apply to the set of tensors $\underset{\sim}{V}^{(k)}(A,B)$ under the operators of U_X. The branching rule

$$\{21^{X-2}0\} \rightarrow [2] + [11] \tag{4.25}$$

is then required.

The transformation properties of the two-particle states and single particle operators have been found to be very similar. When states of operators are coupled care must be taken to ensure correct normalization. We could therefore adopt the combinations

$$\frac{1}{\sqrt{2}}|AB\kappa k\pi q\rangle^{\pm} \quad \text{and} \quad \frac{1}{\sqrt{2}}\overset{\pm}{W}{}^{(\kappa k)}_{\pi q}(A,B) \qquad (A \neq B) \tag{4.26}$$

and

$$\tfrac{1}{2}|AA\kappa k\pi q\rangle^{\pm} \equiv |AA\kappa k\pi q\rangle \quad \text{and} \quad \tfrac{1}{2}\overset{\pm}{W}{}^{(\kappa k)}_{\pi q}(A,A) \equiv W^{(\kappa k)}_{\pi q}(AA) \tag{4.27}$$

An example of the use of coupling the normalized operators for the Coulomb interaction in the R_4 scheme will be given in Chapter 6.

7. GENERAL CLASSIFICATION SCHEMES

The algebra of the generalized Racah tensors gives a powerful tool for studying the properties of mixed configurations. The nucleon configurations $(s+d)^N$ have been studied by Elliott[38] using the scheme

$$U_{24} \rightarrow SU_4 \times (SU_6 \rightarrow SU_3 \rightarrow R_3)$$

while Feneuille[36] has studied the equivalent problem for electron configurations but using the alternative scheme

$$U_{12} \rightarrow Sp_{12} \rightarrow SU_2 \times (R_6 \rightarrow R_5 \rightarrow R_3).$$

This latter scheme is of dubious physical significance in atoms since it fails to mix the eigenfunctions of the ^1D states of the d^2 and ds configurations which are known to couple strongly.

The chain of groups

$$U_{2n^2} \rightarrow Sp_{2n^2} \rightarrow SU_2 \times (R_{n^2} \rightarrow R_4 \rightarrow R_3) \tag{4.28}$$

is useful in studying electrons moving in a Coulomb field where in the case of the non-relativistic hydrogen atom the orbitals associated with the principal quantum number n are all degenerate. In this scheme the single particle eigenfunctions transform as

$$|\{1\}\langle 1\rangle S[10\cdots 0][n-1,0]LM_S M_L\rangle$$

where $L = 0,1,\cdots,n-1$, and the group labels are written in the order indicated by Eq. (4.28).

In the particular case of $n = 3$ which arises in the classification of the states of the $(3s + 3p + 3d)^n$ configurations we need to use the group scheme

$$U_{18} \rightarrow Sp_{18} \rightarrow SU_2 \times (R_9 \rightarrow R_4 \rightarrow R_3). \tag{4.29}$$

The branching rules for $Sp_{18} \rightarrow SU_2 \times R_9$ and $R_9 \rightarrow O_4$ are given in Appendix III. The latter branching rules are easily evaluated in terms of the plethysm

$$[20] \otimes [\lambda] \equiv (\{2\} - \{0\}) \otimes [\lambda].$$

To complete the classification we note that under $O_4 \rightarrow R_4$

$$[pq]' \rightarrow [pq] + [p-q] \qquad (q > 0)$$

$$[p0]' \rightarrow [p0]$$

while under $R_4 \to R_3$

$$[pq] \to p, p-1, \cdots, |q|.$$

We note that the problem of duplicated R_4 representations in the $R_9 \to R_4$ branching rules becomes appreciable for all but the simplest R_9 representations. The situation will obviously worsen as configurations involving higher values of the principal quantum number n are considered.

8. THE COULOMB INTERACTION

After the states of a mixed configuration have been classified by their transformation properties under a chain of groups it is desirable to partition the Hamiltonian into parts having well-defined transformation properties under the same group chain. We now consider in general terms the Coulomb repulsion.

The Coulomb interaction between electrons may be written in the form[47]

$$H_c = \sum_{i>j}^{N} \frac{e^2}{r_{ij}} = e^2 \sum_{k} \sum_{i>j}^{N} \frac{r_<^k}{r_>^{k+1}} (\underset{\sim}{C}_i^{(k)} \cdot \underset{\sim}{C}_j^{(k)}) \tag{4.30}$$

where

$$\underset{\sim}{C}_i^{(k)} = \sum_{A,B} (-1)^A \begin{pmatrix} A & k & B \\ 0 & 0 & 0 \end{pmatrix} [A,B]^{\frac{1}{2}}[k]^{-\frac{1}{2}} \underset{\sim}{v}_i^{(k)}(A,B)$$

$$= \tfrac{1}{2} \sum_{A,B} (-1)^A \begin{pmatrix} A & k & B \\ 0 & 0 & 0 \end{pmatrix} [A,B]^{\frac{1}{2}}[k]^{-\frac{1}{2}} \tag{4.31}$$

$$(\underset{\sim}{v}_i^{(k)}(A,B) + (-1)^{A-B}\underset{\sim}{v}_i^{(k)}(B,A))$$

Because A+k+B is even we have a sum of operators of the form ${}^{p}\underset{\sim}{v}_i^{(k)}(A,B)$ where p is the parity of k, which is the same as that of A-B.

Using

$$(\underset{\sim}{V}^{(k)}(A,B).\underset{\sim}{V}^{(k)}(C,D) = \sum_{i\neq j} (\underset{\sim}{v}_i^{(k)}(A,B).\underset{\sim}{v}_j^{(k)}(C,D))$$

$$+ \delta(A,D)\delta(B,C)(-1)^{A-B}$$

$$[k][A]^{-\frac{1}{2}} V_0^{(0)}(A,A) \tag{4.32}$$

we obtain

$$H_c = \tfrac{1}{4} \sum_k \sum_{A,B,C,D} R^{(k)}(AB;CD)(-1)^{A+B}[A,B,C,D]^{\frac{1}{2}}[k]^{-1}$$

$$\times \begin{pmatrix} A & k & C \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} B & k & D \\ 0 & 0 & 0 \end{pmatrix} [\,({}^{p}\underset{\sim}{V}^{(k)}(A,C).{}^{p}\underset{\sim}{V}^{(k)}(B,D))$$

$$- 2\delta(A,D)\delta(B,C)\ V_0^{(0)}(A,A)] \tag{4.33}$$

where the $R^{(k)}(AB;CD)$'s are the usual Condon and Shortley radial integrals.

For a set of configurations involving orbitals of the same parity all of the operators appearing in Eq. (33) are of the form $\overset{+}{\underset{\sim}{V}}{}^{(k)}(A,B)$ which transform like the antisymmetric two-particle states constructed from the same set of orbitals. This result is entirely analogous to that known for a single configuration. However, for configurations involving orbitals of differing parities we have also the set of tensors $\overset{-}{\underset{\sim}{V}}{}^{(k)}(A,B)$ $(A \neq B)$ to consider. These tensors, unlike those of $\overset{+}{\underset{\sim}{V}}{}^{(k)}(A,B)$, are generators of the group R_X and as such preserve the representation label of R_X as a "good" quantum number.

CHAPTER 5

COUPLING COEFFICIENTS

1. THE n-j SYMBOLS

The ideas of coupling together two or more angular momenta are well known[27,46,48]. The coupling coefficients, often known as Clebsch-Gordan Coefficients, have been studied at length and various methods have evolved for handling sums and products of them. The most powerful is a graphical technique that takes the phases into account, expounded by Jucys et al.[43]. Their book does not, however, include a summary of the rules and so I give the more useful rules in Table VI.

2. GENERALIZED COUPLING COEFFICIENTS

The coupling coefficient for vectors $|LM\rangle$, where L is an R_3 representation label and where M specifies which of the 2L+1 kets of the representation we have, may be generalized to any group chain[49-54]. We write

$$|(W_1W_2)\gamma WM\rangle = \sum_{M_1M_2} \langle W_1M_1;W_2M_2|\gamma WM\rangle|W_1M_1\rangle|W_2M_2\rangle \tag{5.1}$$

The labels WM completely specifies the symmetry of the state and the number γ is required since the Kronecker product

$W_1 \times W_2$ may include W more than once. The properties of the coefficients defined by eqn (5.1) have been studied by Derome[49]. The coefficients have essentially the symmetry of the ordinary R_3 symbols for simply reducible groups (γ=1, only), but for other groups, several complications occur with respect to the choice of phases.

It is more useful, physically, to regard the M label of $|LM\rangle$ as a representation label of R_2, and to redefine the group coupling coefficients for a chain of groups, i.e. to extend the chain $R_3 \to R_2$ to some other (longer) chain. In order to show the properties of such coefficients, defined with respect to any chain, I use kets $|WULM\rangle$ defined on four groups, and require that the two smallest groups, (giving rise to the representations labels L and M) be simply reducible. In the ket $|WULM\rangle$ we may require additional labels α and β to completely specify the ket since the branchings may give rise to multiplicities. However, I shall include these labels in the respective representation labels for the sake of clarity.

$$|W\alpha U\beta LM\rangle \equiv |WULM\rangle .$$

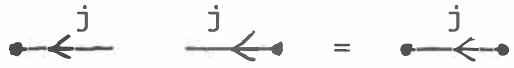
Likewise in coupling kets additional labels γ may be required as in eqn (5.1) but these too will be omitted.

The coupling equation becomes

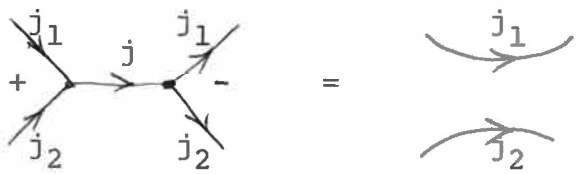
TABLE VI: Graphical Coupling Techniques

Rules

1) A summation over m requires a factor of $(-1)^{j-m}$ and to join free ends. The arrows must follow:

$\Sigma_m (-1)^{j-m}$ 

2) A summation over j requires a factor of (2j+1). Leave out the lines j and join ends of the free lines formed, to corresponding nodes. Corresponding nodes have the lines in the same cyclic order, but with arrows in opposite directions

e.g. Σ_j 

N.B. We may have A-A' or A-B, A'-B' etc. all joined by j, the single summation line.

3) Change of cyclic order of a node $(j_1 j_2 j_3)$ introduces a phase of $(-1)^{j_1+j_2+j_3}$.

4) Change of direction of a closed line j introduces $(-1)^{2j}$.

5) Can merge identical nodes, or separate on three lines

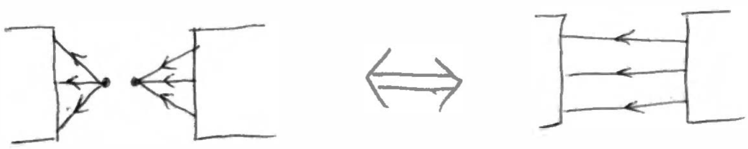
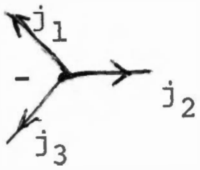


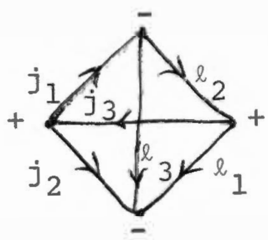
TABLE VI (contd)

Basic Figures

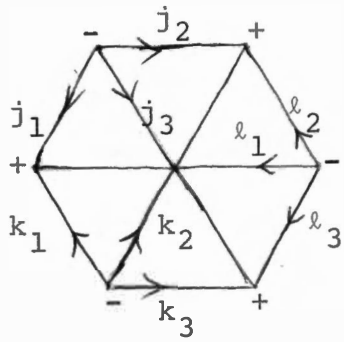
$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} =$



$\begin{Bmatrix} j_1 & j_2 & j_3 \\ \ell_1 & \ell_2 & \ell_3 \end{Bmatrix} =$



$\begin{Bmatrix} j_1 & j_2 & j_3 \\ \ell_1 & \ell_2 & \ell_3 \\ k_1 & k_2 & k_3 \end{Bmatrix} =$



$$|(W_1W_2)WULM\rangle = \sum_{U_1L_1M_1U_2L_2M_2} \langle W_1U_1L_1M_1;W_2U_2L_2M_2|WULM\rangle$$

$$|W_1U_1L_1M_1\rangle|W_2U_2L_2M_2\rangle \qquad (5.2)$$

A lemma due to Racah[1] allows the coefficient to be factorized:

$$\langle W_1U_1L_1M_1;W_2U_2L_2M_2|WULM\rangle = \langle W_1U_1;W_2U_2|WU\rangle\langle U_1L_1;U_2L_2|UL\rangle$$

$$\langle L_1M_1;L_2M_2|LM\rangle \qquad (5.3)$$

A similar expansion is made for the bra $\langle(W_1W_2)WULM|$ and combination with eqn (5.2) leads to the orthogonality relations

$$\sum_{M_1M_2} \langle L_1M_1;L_2M_2|LM\rangle\langle L'M'|L_1M_1;L_2M_2\rangle = \delta(MM')\delta(LL') \qquad (5.4)$$

$$\sum_{L_1L_2} \langle U_1L_1;U_2L_2|UL\rangle\langle U'L'|U_1L_1;U_2L_2\rangle = \delta(UU') \qquad (5.5)$$

$$\sum_{U_1U_2} \langle W_1U_1;W_2U_2|WU\rangle\langle W'U'|W_1U_1;W_2U_2\rangle = \delta(WW') \qquad (5.6)$$

It is interesting to note that the $\delta(MM')$ in eqn (5.4) comes from the fact that M is unique, given M_1 and M_2, and that it is not a consequence of the orthogonality relations.

From the orthogonality relations and eqn (5.2) it follows that

$$|W_1U_1L_1M_1\rangle|W_2U_2L_2M_2\rangle = \sum_{WULM} \langle WULM|W_1U_1L_1M_1;W_2U_2L_2M_2\rangle$$

$$|(W_1W_2)WULM\rangle \qquad (5.7)$$

Multiplication by $|W_1U_1'L_1'M_1'\rangle|W_2U_2'L_2'M_2'\rangle$ and its corresponding expansion leads to

$$\sum_W \langle W_1U_1;W_2U_2|WU\rangle\langle W_1U_1';W_2U_2'|WU\rangle = \delta(U_1U_1')\delta(U_2U_2') \qquad (5.8)$$

$$\sum_U \langle U_1L_1;U_2L_2|UL\rangle\langle U_1L_1';U_2L_2'|UL\rangle = \delta(L_1L_1')\delta(L_2L_2') \qquad (5.9)$$

$$\sum_{LM} \langle L_1M_1;L_2M_2|LM\rangle\langle L_1M_1';L_2M_2'|LM\rangle = \delta(M_1M_1')\delta(M_2M_2') \qquad (5.10)$$

where, of course, in eqn (5.10) only one term in the sum over M will be non-zero.

The coupling coefficient $\langle W_1U_1;W_2U_2|WU\rangle$ has certain symmetry properties. It will be zero unless $W_1 \times W_2 \supset W$ and $U_1 \times U_2 \supset U$ where 'x' denotes the Kronecker product of the representations. Owing to the symmetry of the Kronecker product (see eqn (3.50)), it is seen that the symmetry would be better displayed by use of a symbol $(W_1U_1,W_2U_2,W^*U^*|0)$. In fact if we write

$$(W_1U_1,W_2U_2,W^*U^*|0) = (f(U)/f(W))^{\frac{1}{2}}\langle W_1U_1;W_2U_2|WU\rangle \qquad (5.11)$$

it can be seen that from Racah's theorem[1] a permutation of the representation pairs will only produce a phase factor. This phase factor is given algebraically for the R_3-R_2

coefficient[48]; and the introduction of the factor $(-1)^{j_1-j_2+m}$ leads to the usual symmetries of the 3j symbol. Similar symmetries occur for the R_4-R_3 coefficient[50]. However, Derome and Sharp[51] have shown that for groups that are not simply reducible, it is impossible to choose a unique phase in this manner.

3. GENERALIZED RECOUPLING COEFFICIENTS

The 6j symbol is related to the overlap between the two possible ways of coupling together three angular momenta. I generalize this for all group chains.

We write the two states as:

$$|(W_1W_2)W'W_3WULM\rangle \quad \text{and} \quad |W_1(W_2W_3)\overline{W}\ WULM\rangle \tag{5.12}$$

By the Wigner Eckart theorem, the dependence of U, L and M is entirely contained in the kets, hence:

$$|(W_1W_2)W'W_3WULM\rangle = \sum_{\overline{W}}\langle W_1(W_2W_3)\overline{W}W|(W_1W_2)W'W_3W\rangle \; |W_1(W_2W_3)\overline{W}\ WULM\rangle \tag{5.13}$$

The orthogonal relation follows

$$\sum_{W'}\langle(W_1W_2)W'W_3W|W_1(W_2W_3)\overline{W}W\rangle\langle W_1(W_2W_3)\tilde{W}W|(W_1W_2)W'W_3W\rangle = \delta(\overline{W}\tilde{W}) \tag{5.14}$$

Both sides of eqn (5.13) may be expanded in the form

$$|(W_1W_2)W'W_3WULM\rangle = \sum_{U_1L_1M_1} \sum_{U_2L_2M_2} \sum_{U_3L_3M_3} \sum_{U'L'M'}$$

$$\langle W_1U_1L_1M_1;W_2U_2L_2M_2|W'U'L'M'\rangle\langle W'U'L'M';W_3U_3L_3M_3|WULM\rangle$$

$$|W_1U_1L_1M_1\rangle|W_2U_2L_2M_2\rangle|W_3U_3L_3M_3\rangle \qquad (5.15)$$

Equating coefficients of the simple states eqn (5.13) leads to a sum over $U'L'M'$ on the left and a sum over $\overline{W}\ \overline{U}\ \overline{L}\ \overline{M}$ on the right.

Factorizing the coupling coefficients and multiplying by

$$\sum_{M_2M_3} \langle L_2M_2;L_3M_3|\overline{L}'\overline{M}'\rangle$$

and then for L_2 L_3 etc., we are led to the recoupling equation

$$\langle W_1U_1;\overline{W}\ \overline{U}|WU\rangle\langle(W_1W_2)W'W_3W|W_1(W_2W_3)\overline{W}W\rangle$$

$$= \sum_{U'U_2U_3} \langle W_2U_2;W_3U_3|\overline{W}\ \overline{U}\rangle\langle W_1U_1;W_2U_2|W'U'\rangle\langle W'U';W_3U_3|WU\rangle$$

$$\langle(U_1U_2)U'U_3U|U_1(U_2U_3)\overline{U}U\rangle \qquad (5.16)$$

If $W \equiv L$ and $U \equiv M$ then the overlap integral in U is 1 and we are led to the usual expression of a 6j in terms of a product of 3j symbols. Use of symmetry property (5.11) in

(5.16) leads to symmetries with respect to interchange of the order of the representations similar to those well known for the 6j overlap integral[48].

4. FRACTIONAL PARENTAGE COEFFICIENTS

In the previous chapter various possible group chains were discussed for atomic shell theory. We shall here limit ourselves to the LS coupled case:

$$U_{2X} \rightarrow Sp_{2X} \rightarrow SU_2 \times [R_X \rightarrow \cdots \rightarrow R_3 \rightarrow R_2] \qquad (5.17)$$

The states are specified by the set of quantum numbers $|\{l^n\}\langle l^\nu \rangle W S \gamma L M_L M_S\rangle$ where W is a representation of R_X of the form $[2^a 1^b]^\sigma$ and γ the quantum number of any group(s) nested between R_X and R_3. We have $a = \frac{v}{2} - S$, b = minimum of 2S, X-v. (5.18)

and σ gives which one of the two conjugate characters of $R_{2\nu}$ it is when $a+b = \nu$.

A coefficient of fractional parentage (cfp) is usually defined as a specialized coupling coefficient. We couple a single electron onto a state of n-1 electrons:

$$|nvS_1W\gamma LM_LM_S\rangle = \Sigma \langle \bar{S}\ \bar{M}_S, sm_s|SM_S\rangle\langle \bar{L}\ \bar{M}_L\ \ell m_\ell|LM_L\rangle$$

$$\langle n-1,\bar{v}\ \bar{S}\ \bar{W}\ \bar{\gamma}\ \bar{L} + \ell |\} nvSW\gamma LM_LM_S\rangle\ |n-1,\bar{v}\ \bar{S}\ \bar{W}\ \bar{\gamma}\ \bar{L}\ \bar{M}_L\bar{M}_S\rangle|\ell m_\ell m_s\rangle \quad (5.]$$

The cfp is more useful factorized:

$$\langle n-1,\bar{v}\ \bar{S}\ \bar{W}\ \bar{\gamma}\ \bar{L} + \ell|\}nvSW\gamma L\rangle$$

$$= \langle\{1^{n-1}\}\langle 1^{\bar{v}}\rangle;\{1\}\langle 1\rangle|\{1^n\}\langle 1^v\rangle\rangle.\langle\langle 1^{\bar{v}}\rangle\bar{S}\ \bar{W};\langle 1\rangle^2[1]|$$

$$\langle 1^v\rangle SW\rangle\langle\bar{W}\ \bar{\gamma}\ \bar{L},[1]\ell|W\gamma L\rangle \qquad (5.20)$$

Use of the reduced matrix element of $\underset{\sim}{S}$[48] and properties of eqn (4.6) and eqn (5.11) leads easily to formulae for the $U_{2X} \rightarrow Sp_{2X}$ and $Sp_{2X} \rightarrow SU_2 \times R_X$ factors of eqn (5.20), although no phase information is available. The results are given in Table VII.

Two electron cfp are of interest. The equations used for the above are not sufficient but the recoupling equation, eqn (5.16), may be used together with the various properties of the overlap integrals for the two spaces. After considerable algebraic manipulation I arrive at Table VIII.

I have not discussed the second quantization approach[55], for although it gives many of the equations, it does not give them all. The approach also confuses simple group theoretic properties of this chain of groups, with other electronic properties. For instance it is not clear, using the second quantization approach, that the coupling coefficients are independent of the nature of the mixed configuration.

TABLE VII: One Electron Factorized CFP

Writing $T = 2S+1$, $w = 2X+2-v$

$U_{2X} \rightarrow Sp_{2X}$

$$\langle n-1,v-1;1,1|nv\rangle^2 = \frac{v}{n} \cdot \frac{w-n}{w-v}$$

$$\langle n-1,v+1;1,1|nv\rangle^2 = \frac{w}{n} \cdot \frac{n-v}{w-v}$$

$Sp_{2X} \rightarrow SU_2 \times R_X$

$$\langle v-1,S-\tfrac{1}{2};1,\tfrac{1}{2}|vS\rangle^2 = \frac{T-1}{2T} \cdot \frac{v+T+1}{v}$$

$$\langle v-1,s+\tfrac{1}{2};1,\tfrac{1}{2}|vS\rangle^2 = \frac{T+1}{2T} \cdot \frac{v-T+1}{v}$$

$$\langle v+1,S-\tfrac{1}{2};1,\tfrac{1}{2}|vS\rangle^2 = \frac{T-1}{2T} \cdot \frac{w+T+1}{w}$$

$$\langle v+1,S+\tfrac{1}{2};1,\tfrac{1}{2}|vS\rangle^2 = \frac{T+1}{2T} \cdot \frac{W-T+1}{w}$$

TABLE VIII: Two Electron Factorized CFP

$U_{2X} \rightarrow Sp_{2X}$

$$\langle n-2,v-2;2,2|nv\rangle^2 = \frac{v}{n} \cdot \frac{v-1}{n-1} \cdot \frac{w-n}{w-v} \cdot \frac{w-n+2}{w-v+2}$$

$$\langle n-2,v\ \ ;2,2|nv\rangle^2 = 2\,\frac{w}{n} \cdot \frac{v}{n-1} \cdot \frac{w-n}{w-v-2} \cdot \frac{w-v}{w-v+2} \cdot \frac{w+v}{w+v-2}$$

$$\langle n-2,v+2;2,2|nv\rangle^2 = \frac{w}{n} \cdot \frac{w-1}{n-1} \cdot \frac{n-w}{w-v} \cdot \frac{n-v-2}{w-v-2}$$

$$\langle n-2,v\ \ ;2,0|nv\rangle^2 = \frac{1}{n} \cdot \frac{n-v}{n-1} \cdot \frac{w-n}{w+v-2}$$

$Sp_{2X} \rightarrow SU_2 \times R_X$

$$\langle v-2,S;2,0|vS\rangle^2 = \tfrac{1}{4} \cdot \frac{v+T+1}{v} \cdot \frac{v-T+1}{v-1}$$

$$\langle v,\ \ S;2,0|vS\rangle^2 = \tfrac{1}{4} \cdot \frac{(w+v-2)(wv-T^2+1) + 8wv}{w.v(w+v)}$$

$$\langle v+2,S;2,0|vS\rangle^2 = \tfrac{1}{4} \cdot \frac{w+T+1}{w} \cdot \frac{w-T+1}{w-1}$$

$$\langle v-2,S-1;2,1|vS\rangle^2 = \frac{T-2}{4T} \cdot \frac{v+T+1}{v} \cdot \frac{v+T-1}{v-1}$$

$$\langle v-2,S;2,1|vS\rangle^2 = \tfrac{1}{4} \cdot \frac{v+T+1}{v} \cdot \frac{v-T+1}{v-1}$$

$$\langle v-2,S+1;2,1|vS\rangle^2 = \frac{T+2}{4T} \cdot \frac{v-T+1}{v} \cdot \frac{v-T-1}{v-1}$$

$$\langle v\ \ ,S-1;2,1|vS\rangle^2 = \frac{T-2}{4T} \cdot \frac{v+T+1}{v} \cdot \frac{w+T+1}{w} \cdot \frac{w+v-2}{w+v}$$

TABLE VIII (contd)

$$\langle v\ ,S\ ;2,1|vS\rangle^2 = \tfrac{1}{4}\ .\ \frac{(w+2)(v+2)-(T-1)(T+1)}{v\ w}\quad \frac{w+v-2}{w+v}$$

$$\langle v\ ,S+1;2,1|vS\rangle^2 = \frac{T+2}{4T}\ .\ \frac{v-T+1}{v}\ .\ \frac{w-T+1}{w}\ .\ \frac{w+v-2}{w+v}$$

$$\langle v+2,S-1;2,1|vS\rangle^2 = \frac{T-2}{4T}\ .\ \frac{w+T+1}{w}\ .\ \frac{w+T-1}{w-1}$$

$$\langle v+2,S\ ;2,1|vS\rangle^2 = \tfrac{1}{4}\ .\ \frac{w+T+1}{w}\ .\ \frac{w-T+1}{w-1}$$

$$\langle v+2,S+1;2,1|vS\rangle^2 = \frac{T+2}{4T}\ .\ \frac{w-T+1}{w}\ .\ \frac{w-T-1}{w-1}$$

It is to be noted that for v or 2s = 0 or 1 some of these coefficients are zero, but their formulae give rise to negative values. For this case others will be twice the value given.

The phases of these coefficients are very largely undefined. Racah[1] makes a choice for $R_{2\ell+1}$ but this choice is not suitable for all groups (e.g. R_4). He obtains restrictions on the phases knowing the phase for one subgroup (SU_2) and requiring no phase to arise in the rotation group when using eqn (5.11). This choice would obviously not be satisfactory for the rotation group R_4 where permutation of the order of representations in

$$\langle [p_1q_1]\ell_1; [p_2q_2]\ell_2 | [p_3q_3]\ell_3 \rangle$$

introduces a phase of $(-1)^{p_1+p_2+p_3}$. Thus until all possible restrictions are found it does not seem worthwhile making a phase choice.

CHAPTER 6

APPLICATIONS TO THE $(s+p)^N$ SHELL

1. INTRODUCTION

It is well known that the energy levels of a hydrogen atom, in the non-relativistic approximation, may be grouped in the series

$$1s;\ 2s2p;\ 3s3p3d;\ 4s4p4d;\ \cdots \tag{6.1}$$

with orbitals having the same principal quantum number n having total degeneracy n^2. Fock[56] and Bargman[57] have shown that for the bound states of a single electron moving in a pure coulomb potential, the group appropriate to the symmetry description of the Hamiltonian is the rotation group in four dimensions, R_4. Indeed the orbital eigenfunctions associated with principal quantum number n span the n^2 dimensional representation $[n-1,0]$ of R_4. Perelomov and Popov[58] have shown that symmetry of the continuous spectra of the hydrogen atom may be described in terms of the non-compact homogeneous Lorentz group O(3,1). Here we shall restrict our attention to bound states only and thus only R_4 will be considered.

It is of some interest to examine the role of the R_4 group, if any, in the many electron theory of atoms. In

Layzer's[59-61] development of the theory of complex spectra the "complex of configurations" involving a definite set of principal quantum numbers n and parity played a central role. His definition of a complex derives ultimately from the degeneracies associated with the hydrogen atom. Moshinsky[62], following upon the work of Biedenharn[50], has suggested that the group R_4 could be used as a starting poin for treating the electron correlation problem. Wulfman[63] has suggested that the doubly excited helium metastable states, sudied by Lipsky and Russek[64], may be usefully labelled according to the representations of the group R_4.

More recently Alper and Sinanoglu[65,66] have made a detailed study of the role of the group R_4 in the many-electron-theory of atomic structure giving particular attention to the Coulomb interaction in the $(2s+2p)^N$ and $(3s+3p+3d)^N$ configurations. They have concluded that the group R_4 does indeed have relevance as an approximate symmetry in many electron systems and that it clearly exposes the Z and N dependence of the nondynamical electron correlation.

In the present Chapter I wish to examine the significance of the R_4 group as an approximate symmetry group for the Coulomb interaction of a many-electron system. I shall first give a systematic treatment of the group-theoretical properties of the Coulomb interaction in the $(2s+2p)^N$ complex correcting a number of significant errors of substance in the original work of Alper and Sinanoglu and then consider the question "Is the group R_4 an approximate symmetry for many electron theory?"

2. CONSTRUCTION OF R_4 SYMMETRIZED STATES

The states of the $(2s+2p)^N$ complexes may be uniquely labelled by the scheme of quantum numbers

$$|(2s+2p)^N[pq]SLM_SM_L\rangle,$$

or suppressing the quantum numbers M_S M_L, the terms are specified by

$$|(2s+2p)^N[pq]SL\rangle. \qquad (6.1)$$

We first note that the matrix elements of a scalar two particle operator $G = \sum_{i>j}^{N} g_{ij}$ between states of any N electron complex X^N, where $X \equiv \ell_1 + \ell_2 + \cdots + \ell_k$, may be expressed as a linear combination of two electron matrix elements in X^2 weighted by the appropriate two-particle coefficients of fractional parentage to give

TABLE IX: R_4 Symmetrized Eigenfunctions of $(2s+2p)^1$ and $(2s+2p)^2$.

$$|[10]\,^2P\rangle = -\,|2s\ ^2P\rangle$$

$$|[10]\,^2S\rangle = +\,|2p\ ^2S\rangle$$

$$|[11]\,^3P\rangle = \frac{1}{\sqrt{2}}\left(|2p^2\ ^3P\rangle + |2s2p\ ^3P\rangle\right)$$

$$|[1\text{-}1]\,^3P\rangle = \frac{1}{\sqrt{2}}\left(|2p^2\ ^3P\rangle - |2s2p\ ^3P\rangle\right)$$

$$|[20]\,^1D\rangle = |2p^2\ ^1D\rangle$$

$$|[20]\,^1P\rangle = -\,|2s2p\ ^1P\rangle$$

$$|[20]\,^1S\rangle = \frac{\sqrt{3}}{2}\,|2s^2\ ^1S\rangle - \tfrac{1}{2}|2p^2\ ^1S\rangle$$

$$|[00]\,^1S\rangle = \tfrac{1}{2}|2s^2\ ^1S\rangle + \frac{\sqrt{3}}{2}\,|2p^2\ ^1S\rangle$$

$$\langle X^N_\alpha[pq]SL|G|X^N_{\alpha'}[pq]'SL\rangle$$

$$= \frac{N(N-1)}{2} \sum_{[\overline{pq}]\bar{S}\bar{L}} \sum_{[pq]'',[pq]'''S''L''} \langle X^N_\alpha[pq]SL\{|X^{N-2}[\overline{pq}]\bar{S}\bar{L};X^2[pq]''S''\rangle$$

$$\times\langle X^2[pq]''S''L''|g_{12}|X^2[pq]'''S''L''\rangle$$

$$\times\langle X^{N-2}[\overline{pq}]\bar{S}\bar{L};X^2[pq]'''S''L''|\}X^N_{\alpha'}[pq]'SL\rangle. \qquad (6.2)$$

Inspection of the above equation indicates that R_4 symmetry can only be conserved in X^N if the scalar interaction g_{12} is diagonalized in the two-electron basis $|X^2[pq]SL\rangle$. Thus the question "is the group R_4 an approximate symmetry in many-electron theory?" can be answered by investigating the structure of the X^2 configuration alone.

The states symmetrized according to the scheme of eqn (6.1) may be expanded as a linear combination of the usual single configuration states. The relevant linear combination may be readily determined either by use of Biedenharn's formula for the R_4 Wigner coefficients[50] or by use of his result for the reduced matrix elements of the operator $A^{(1)}$ defined by Eq. (4.11). Either method readily yields the results of Table IX for the (2s+2p) and $(2s+2p)^2$ complexes. The phases defined in Biedenharn's paper are identical to those of Condon and Shortley[47]. It is important to notice that with this convention, the phases of the one electron states in the R_4 scheme are not simply those of conventional orbitals. Our results differ from those of Wulfman[63] and of Alper and Sinanoglu[65,66] due in the first case to a numerical error and in the second to an incorrect choice of group generators and in the transcription of Biedenharn's results. The difference in phase for the linear combinations of the $|[20]^1S\rangle$ and $|[00]^1S\rangle$ states is of critical importance in assessing the relevance of R_4 symmetry in many-electron theory since these are the only states belonging to different R_4 representations that can interact in $(2s+2p)^2$ and thus give rise to a configuration mixing.

We note that the states $|[11]^3P\rangle$ and $|[1-1]^3P\rangle$ involve a linear combination of <u>odd</u> and <u>even</u> parity states. However, we may always form states of well defined parity by forming the linear combinations

$$|[pq]'SL\rangle^{\pm} = \frac{1}{\sqrt{2}}\left(|[pq]SL\rangle \pm |[p-q]SL\rangle\right) \quad (q>0) \quad (6.3)$$

There is no difficulty in obtaining the appropriate linear combinations for more complex two-electron configurations. At this point it should be noted that the linear combinations given by Alper and Sinanoglu[65] for $(3s+3p+3d)^2$ while forming an orthonormal set do not have consistently defined phases.

3. R_4 SYMMETRIZATION OF THE COULOMB INTERACTION

In Chapter 4 we derived the transformation properties of the double-tensor operators $\underset{\sim}{w}^{(\kappa k)}(A,B)$ under all the groups of interest here. In Table X we give the transformation properties of the operators using the abbreviation

$$\overset{\pm}{\underset{\sim}{w}}{}^{(\kappa k)}(\ell,\ell') = \frac{1}{\sqrt{2}}[\underset{\sim}{w}^{(\kappa k)}(\ell,\ell') \pm (-1)^{\kappa+k+\ell-\ell'}\underset{\sim}{w}^{(\kappa k)}(\ell',\ell)]$$

Now the Coulomb interaction may be written

$$\begin{aligned} H_c = \sum_{i>j} & F_0(2s,2s)(\underset{\sim}{v}_i^{(0)}(ss)\cdot\underset{\sim}{v}_j^{(0)}(ss)) \\ & + 3F_0(2p,2p)(\underset{\sim}{v}_i^{(0)}(pp)\cdot\underset{\sim}{v}_j^{(0)}(pp)) \\ & + \sqrt{3}\,F_0(2s,2p)[(\underset{\sim}{v}_i^{(0)}(ss)\cdot\underset{\sim}{v}_j^{(0)}(pp)) + (\underset{\sim}{v}_i^{(0)}(pp)\cdot\underset{\sim}{v}_j^{(0)}(ss))] \\ & + 6\,F_2(2p,2p)(\underset{\sim}{v}_i^{(2)}(pp)\cdot\underset{\sim}{v}_j^{(2)}(pp)) \\ & + 2G_1(2s,2p)(\overset{-}{\underset{\sim}{v}}{}_i^{(1)}(sp)\cdot\overset{-}{\underset{\sim}{v}}{}_j^{(1)}(sp)) \end{aligned} \tag{6.4}$$

The Coulomb interaction as written has well known spin and orbital symmetry - namely scalar- but we wish to split the interaction up into parts of precise R_4 symmetries. This may be done readily as we know the symmetry of the single operators and the R_4-Wigner coefficients[50]. When coupling, the sum is over all subgroup representations and thus we must introduce $\overset{+}{\underset{\sim}{v}}{}^{(1)}(sp)$ and $\underset{\sim}{v}^{(1)}(pp)$.

TABLE X: Symmetrization of One Particle Tensor Operators for $(s+p)^N$.

U_8	Sp_8	$SU_2 \times R_4$	$SU_2 \times R_3$	Symmetrized Operator
$\{21^6\}$	$\langle 1^2 \rangle$	$^3[11]$	^3P	$\frac{1}{\sqrt{2}}[\underset{\sim}{w}^{(11)}(pp) + \overset{+}{\underset{\sim}{w}}{}^{(11)}(sp)]$
		$^3[1\text{-}1]$	^3P	$\frac{1}{\sqrt{2}}[\underset{\sim}{w}^{(11)}(pp) - \overset{+}{\underset{\sim}{w}}{}^{(11)}(sp)]$
		$^1[20]$	^1D	$\underset{\sim}{w}^{(02)}(pp)$
			^1P	$-\overset{+}{\underset{\sim}{w}}{}^{(01)}(sp)$
			^1S	$\frac{\sqrt{3}}{2}\underset{\sim}{w}^{(00)}(ss) - \frac{1}{2}\underset{\sim}{w}^{(00)}(pp)$
	$\langle 2 \rangle$	$^1[11]$	^1P	$\frac{1}{\sqrt{2}}[\underset{\sim}{w}^{(01)}(pp) + \overset{-}{\underset{\sim}{w}}{}^{(01)}(sp)]$
		$^1[1\text{-}1]$	^1P	$\frac{1}{\sqrt{2}}[\underset{\sim}{w}^{(01)}(pp) - \overset{-}{\underset{\sim}{w}}{}^{(01)}(sp)]$
		$^3[20]$	^3D	$\underset{\sim}{w}^{(12)}(pp)$
			^3P	$-\overset{-}{\underset{\sim}{w}}{}^{(11)}(sp)$
			^3S	$\frac{\sqrt{3}}{2}\underset{\sim}{w}^{(10)}(ss) - \frac{1}{2}\underset{\sim}{w}^{(10)}(pp)$
		$^3[00]$	^3S	$\frac{1}{2}\underset{\sim}{w}^{(10)}(ss) + \frac{\sqrt{3}}{2}\underset{\sim}{w}^{(10)}(pp)$
$\{0\}$	$\langle 0 \rangle$	$^1[00]$	^1S	$\frac{1}{2}\underset{\sim}{w}^{(00)}(ss) + \frac{\sqrt{3}}{2}\underset{\sim}{w}^{(00)}(pp)$

The operators ε_k and e_k symmetrized with respect to R_3 and R_4 are given in Tables XI and XII. The possible symplectic group symmetries for these operators are also given. They may be derived using the appropriate plethysms.

Writing

$$H_c = \sum_{k=0}^{6} e_k E_k \tag{6.5}$$

and comparing this with eqn (6.4) we may solve for the coefficients E_k in terms of the Slater integrals (Table XIII) Contrary to Alper and Sinanoglu[65], we note that the exploitation of the R_4 symmetry does not lead to any reduction in the number of parameters required to characterize the Coulomb field. This invalidates the results of their Tables III and V.

This process of symmetrizing with respect to higher groups can be carried out whenever we know the coupling coefficients. The operators must have a common normalization for this procedure and for this reason the factor required for the normalization of the operators is included in Table XII.

4. MATRIX ELEMENTS FOR $(2s+2p)^2$

The matrix elements for the e_k may be readily calculated using standard methods to give the results of Table XIV. We note we may factorize the matrix element of e_i as

TABLE XI: R_3 Symmetrized Operators

$$\varepsilon_0 = \sum_{i>j} (\underset{\sim}{v}_i^{(0)}(ss) \cdot \underset{\sim}{v}_j^{(0)}(ss))$$

$$\varepsilon_1 = \sum_{i \neq j} (\underset{\sim}{v}_i^{(0)}(ss) \cdot \underset{\sim}{v}_j^{(0)}(pp))$$

$$\varepsilon_2 = \sum_{i>j} (\underset{\sim}{v}_i^{(0)}(pp) \cdot \underset{\sim}{v}_j^{(0)}(pp))$$

$$\varepsilon_3 = \sum_{i>j} (\overset{+}{\underset{\sim}{v}}{}^{(1)}(sp) \cdot \overset{+}{\underset{\sim}{v}}{}^{(1)}(sp))$$

$$\varepsilon_4 = \sum_{i>j} (\underset{\sim}{v}_i^{(2)}(pp) \cdot \underset{\sim}{v}_j^{(2)}(pp))$$

$$\varepsilon_5 = \sum_{i>j} (\overset{-}{\underset{\sim}{v}}{}_i^{(1)}(sp) \cdot \overset{-}{\underset{\sim}{v}}{}_j^{(1)}(sp))$$

$$\varepsilon_6 = \sum_{i>j} (\underset{\sim}{v}_i^{(1)}(pp) \cdot \underset{\sim}{v}_j^{(1)}(pp))$$

TABLE XII: R_4 Symmetrized Operators

Sp_8	R_4	^{2S+1}L	normalization	
$\langle 0\rangle$	[00]	^1S	$\frac{1}{2}$	$e_0 = \varepsilon_0+\sqrt{3}\varepsilon_1+3\varepsilon_2$
$\langle 22\rangle+\langle 0\rangle$	[00]	^1S	$\frac{1}{6}$	$e_1 = 3\varepsilon_0-\sqrt{3}\varepsilon_1+\varepsilon_2-4\varepsilon_3+4\varepsilon_4$
$\langle 22\rangle+\langle 0\rangle$	[00]	^1S	$\frac{1}{\sqrt{3}}$	$e_2 = 2\varepsilon_6+2\varepsilon_5$
$\langle 11\rangle$	[20]	^1S	$\frac{1}{2\sqrt{3}}$	$e_3 = 3\varepsilon_0+\sqrt{3}\varepsilon_1-3\varepsilon_2$
$\langle 22\rangle+\langle 11\rangle$	[20]	^1S	$\frac{1}{2\sqrt{3}}$	$e_4 = 3\varepsilon_0-\sqrt{3}\varepsilon_1+\varepsilon_2-2\varepsilon_3-2\varepsilon_4$
$\langle 22\rangle+\langle 11\rangle$	[20]	^1S	$\frac{1}{2\sqrt{3}}$	$e_5 = 2\varepsilon_6-2\varepsilon_5$
$\langle 22\rangle$	[40]	^1S	$\frac{1}{6\sqrt{5}}$	$e_6 = 15\varepsilon_0-5\sqrt{3}\varepsilon_1+5\varepsilon_2+10\varepsilon_3+2\varepsilon_4$

TABLE XIII: Radial Coefficients for R_4 Symmetry

$$E_0 = \frac{1}{16}[F_0(2s2s) + 6F_0(2s2p) + 9F_0(2p2p)]$$

$$E_1 = \frac{1}{48}[F_0(2s2s) - 2F_0(2s2p) + F_0(2p2p) + 40F_2(2p2p)]$$

$$E_2 = \tfrac{1}{2}G_1(2s2p)$$

$$E_3 = \frac{1}{8}[F_0(2s2s) + 2F_0(2s2p) - 3F_0(2p2p)]$$

$$E_4 = \frac{1}{16}[F_0(2s2s) - 2F_0(2s2p) + F_0(2p2p) - 20F_2(2p2p)]$$

$$E_5 = -\tfrac{1}{2}G_1(2p2p)$$

$$E_6 = \frac{1}{48}[F_0(2s2s) - 2F_0(2s2p) + F_0(2p2p) + 4F_2(2p2p)]$$

$$E_7 = \tfrac{1}{4}[I(2s) + 3I(2p) + 2F_0(1s2s) + 6F_0(1s2p) - G_0(1s2s) - 3G_1(1s2p)]$$

$$E_8 = \tfrac{1}{4}[I(2s) - I(2p) + 2F_0(1s2s) - 2F_0(1s2p) - G_1(1s2s) + G_1(1s2p)]$$

TABLE XIV: Matrix elements of $(s+p)^2$

	e_0	e_1	e_2	e_3	e_4	e_5	e_6	e_7	e_8
$\langle [11]\,^3P \mid e_i \mid [11]\,^3P \rangle$	1	-3	-1	·	·	·	·	2	·
$\langle [1\text{-}1]\,^3P \mid e_i \mid [1\text{-}1]\,^3P \rangle$	1	-3	-1	·	·	·	·	2	·
$\langle [11]\,^3P \mid e_i \mid [1\text{-}1]\,^3P \rangle$	·	·	·	-1	2	-1	·	·	-2
$\langle [20]\,^1D \mid e_i \mid [20]\,^1D \rangle$	1	1	1	-1	·	1	2	2	-2
$\langle [20]\,^1P \mid e_i \mid [20]\,^1P \rangle$	1	1	1	1	·	-1	-10	2	2
$\langle [20]\,^1S \mid e_i \mid [20]\,^1S \rangle$	1	1	1	2	·	-2	-20	2	4
$\langle [20]\,^1S \mid e_i \mid [00]\,^1S \rangle$	·	·	·	$\sqrt{3}$	$2\sqrt{3}$	$\sqrt{3}$	·	·	$2\sqrt{3}$
$\langle [00]\,^1S \mid e_i \mid [00]\,^1S \rangle$	1	9	-3	·	·	·	·	2	·

$$\langle \gamma_2 W_2 L_2 M_2 | e_i^{WLM} | \gamma_1 W_1 L_1 M_1 \rangle = \langle LM, L_1 M_1 | L_2 M_2 \rangle \langle WL, W_1 L_1 | W_2 L_2 \rangle$$
$$\langle \gamma_2 W_2 || e_i^{W} || \gamma_1 W_1 \rangle \qquad (6.6)$$

Thus reducing the number of calculations required. We have now separated the Hamiltonian into R_4-symmetry preserving $(e_0E_0 + E_1e_1 + E_2e_2)$ and symmetry breaking $(E_3e_3 + E_4e_4 + e_5E_5 + e_6E_6)$ terms. The R_4 model will only be valid if the last part is small. In order to obtain some feeling for the size of the radial integrals we present in Table XV the values of the E_i obtained using either hydrogen-like orbitals or the Hartree-Fock radial integrals found for neutral beryllium by Condon and Odabasi[67].

The ^1S energy levels are of particular interest since the R_4 model gives a prediction of the mixing of the $|2s^2\ ^1S\rangle$ and $|2p^2\ ^1S\rangle$ states. Using the hydrogenic radial integrals the relevant energy matrices in the two schemes are

$\|[20]\ ^1S\rangle$	$\|[00]\ ^1S\rangle$
108	$-16\sqrt{3}$
$-16\sqrt{3}$	80

$\|2p^2\ ^1S\rangle$	$\|2s^2\ ^1S\rangle$
111	$-15\sqrt{3}$
$-15\sqrt{3}$	77

where the matrix elements have units of $Ze^2/512a_0$. In this case the R_4 scheme is less diagonal than the configuration scheme.

TABLE XV: Radial Integrals

	Hydrogenic $Ze^2/512\ a_0$ a.u.	Hartree-Fock† a.u.
E_0	$\frac{1421}{16}$	.3152
E_1	$\frac{73}{48}$	.0047
E_2	$\frac{15}{2}$	.0511
E_3	$-\frac{33}{8}$	.0094
E_4	$-\frac{35}{8}$	$-$ .0061
E_5	$-\frac{15}{2}$	$-$ .0511
E_6	$\frac{41}{240}$	$-$ .00067
E_7	-	$-$ .5444
E_8	-	$-$ .0344

†Derived from Condon and Odabasi[17]

Using the H-F orbitals we obtain

$|[20]\,^2S\rangle$ $\quad |[00]\,^1S\rangle$

0.5054	-0.0933
-0.0933	0.2046

$|2p^2\;^1S\rangle$ $\quad |2s^2\;^1S\rangle$

0.3607	-0.1773
-0.1773	0.3493

in atomic units. Diagonalization of the matrices gives the groundstate eigenfunction for beryllium as

$$
\begin{aligned}
|{}^1S\rangle_0 &= 0.953|[00]\,^1S\rangle + 0.275|[20]\,^1S\rangle \\
&\equiv 0.715|2s^2\;^1S\rangle + 0.700|2p^2\;^1S\rangle \qquad (6.7)
\end{aligned}
$$

suggesting that for these Hartree-Fock orbitals the R_4 scheme is very much better than the configurational scheme.

Multiconfiguration calculations[68-70] for the beryllium atom yield for the groundstate[71]

$$
\begin{aligned}
|{}^1S\rangle_0 &= 0.953|2s^2\;^1S\rangle + 0.299|2p^2\;^1S\rangle \\
&\equiv 0.736|[00]\,^1S\rangle + 0.676|[20]\,^1S\rangle \qquad (6.8)
\end{aligned}
$$

indicating in this case that the configurational scheme is superior. It should be noted that the phase conventions in refs 66 and 70 are unspecified, but evidently opposite to the Condon and Shortley phases[47 & 48]. Comparison of eqns

(6.7) and (6.8) suggests that there is a contradiction between the R_4 and the multi-configuration schemes. To resolve this discrepancy we shall re-examine some of the approximations involved in the R_4 scheme.

5. INCLUSION OF CLOSED SHELL EFFECTS

Equation (6.4) gives a complete description of the Coulomb interaction within the $(2s+2p)^N$ complex but fails to include contributions to the Hamiltonian from the $1s^2$ shell. To take into account these effects for the configuration $1s^2 2s^X 2p^{N-X}$ we must add to eqn (6.4) the terms[47]

$$H'_c = 2I(1s) + F_0(1s1s) + XI(2s) + 2XF_0(1s2s) - XG_0(1s2s)$$
$$+ (N-X)I(2p) + 2(N-X)F_0(1s2p) - (N-X)G_1(1s2p). \quad (6.9)$$

We now express eqn (6.9) as a linear combination of operators having well-defined R_4 symmetry by first noting that the numbers X and N-X may be replaced by their operator equivalents

$$X = V_0^{(0)}(2s2s) \quad \text{and} \quad N-X = \sqrt{3}\, V_0^{(0)}(2p2p)$$

Inspection of Table X shows that we may construct two operators

$$e_7 = V_0^{(0)}(2s2s) + \sqrt{3}\, V_0^{(0)}(2p2p) \quad (6.10a)$$

and

$$e_8 = 3\,V_0^{(0)}(2s2s) - \sqrt{3}\,V_0^{(0)}(2p2p), \qquad (6.10b)$$

having [00] and [20] R_4 symmetry respectively, to give

$$H_c' = 2I(1s) + F_0(1s1s) + e_7E_7 + e_8E_8 \qquad (6.11)$$

where

$$E_7 = \tfrac{1}{4}[I(2s) + 2F_0(1s2s) - G_0(1s2s) + 3I(2p) + 6F_0(1s2p) - 3G_1(1s2p)],$$

and

$$E_8 = \tfrac{1}{4}[I(2s) - I(2p) + 2F_0(1s2s) - 2F_0(1s2p) - G_0(1s2s) + G_1(1s2p)].$$

The first two terms in eqn (6.11) are constant for the terms of a given $(2s+2p)^N$ complex and thus cannot affect the result of eqn (6.7). Similarly, since e_7 is just the number operator with eigenvalues N for all terms of the complex its effect also leaves eqn (6.7) invariant and thus can only alter the absolute energy of the complex.

The term e_8E_8 has [20] symmetry under R_4 and will thus have an off-diagonal matrix between the $|[00]^1S\rangle$ and $|[20]^1S\rangle$ states of $(2s+2p)^2$ as follows from an inspection of Table XIV. The integrals of Condon and Odabasi[67] lead to the values

$$E_7 = -0.5444 \quad \text{and} \quad E_8 = -0.0344 \text{ a.u.}$$

Explicit calculation using these values gives the ground-state eigenfunction of the beryllium atom as

$$|{}^1S\rangle_0' = 0.819|[00]\,{}^1S\rangle + 0.574|[20]\,{}^1S\rangle$$

$$0.907|2s^2\ {}^1S\rangle + 0.413|2p^2\ {}^1S\rangle. \qquad (6.12)$$

This result is more in accord with that of the multi-configuration calculation given in eqn (6.8) and shows that when the $1s^2$ shell effects are included the R_4 scheme ceases to be physical and the configurational scheme becomes superior.

The term e_8E_8 clearly plays a major role in breaking the otherwise good R_4 symmetry. This result might well have been anticipated by noting that in the $(2s+2p)^1$ complex the separation of the ${}^2S$ and ${}^2P$ terms will be, from eqn (6.11) just $-4E_8$. Pure R_4 symmetry would require this splitting to be zero while experimentally we find for the isoelectronic series[71]

	Li I	Be II	B III	C IV	
$-E_8$ =	3725	7985	12095	16150	cm^{-1}
	.0170	.0364	.0551	.0736	a.u.

which is by no means negligible.

6. CONCLUSIONS

My principal result is that the R_4 group does not yield an adequate approximate symmetry scheme for many electron theory. This is contrary to earlier work done[63,65,66], but is in accord with more recent work by Wulfman and Moshinsky[72]. In reaching this conclusion I have eliminated a number of errors in the earlier works and shown that R_4 only approximately diagonalizes the energy matrix when the effects of the inner shells are neglected.

CHAPTER 7

PROGRAMMING CONSIDERATIONS

1. HANDLING PARTITIONS

The operations of the algebra of S-functions, and the use of S-functions in continuous group character analysis, have been largely programmed in FORTRAN IV for an IBM 360/44 computer. All the operations require the handling of large numbers of partitions and techniques must be developed to do this rapidly. We store a partition simply as a vector in two byte (16 binary bit) integer format. A sum of partitions is similarly stored in a rectangular matrix. For the applications to group characters, the S-functions are restricted to having no more parts than the value of the group's dimension. For operations with S-functions we may choose some arbitrary value for the size of the vectors and likewise for the dimensions of the rectangular storage matrices.

A subroutine ORDER was written, using the variable dimension facility of FORTRAN IV, to add such a partition to a matrix of partitions. It was noticed, however, that when calculating the Kronecker product of representations, an inordinate amount of time was spent in this routine. When rewritten, doing the subscripting manually, an incredible saving was produced, in the order of half the total time. Since that time all routines have been written doing the addressing for the compiler, and some of the other more important routines were rewritten.

In all matrices the partitions are ordered in lexical order, largest first but two routines are also used to produce partitions. NEXT produces the next partition of a given number, or the first of the next integer, and LIST produces partitions in lexical order, for the purposes of tabulations.

2. INPUT-OUTPUT

Very little input is required for the programmes. The various main programmes require the group, the group's dimension and where to start and where to stop in a tabulation. A fortran subroutine HEADER reads this information off cards, calculating certain other basic information such as the size of the vectors required. HEADER also initializes an assembler output routine. This routine, DUDLEY, prints only integer and literal information, but divides this into lines and pages, either for the line-printer or the typewriter. The typewriter is used to produce high quality tables with the special brackets and signs required. Owing to the slow speed of the typewriter (10 characters a second) DUDLEY has several output buffers so that the computer can continue calculating while the pages are being typed. The routine PRNT calls DUDLEY with the numbers and brackets required and PRNT also calls a small checking routine that performs a dimensional check on each result.

3. BASIC OPERATIONS

In Chapter 1 I showed how to perform all calculations with just the two basic operations of outer multiplication and division. Two routines KRONK and GAMMA perform these operations in the graphical manner described. All other routines consist of manipulating sums and products of the partitions with the one exception of MONO. This writes an S-function in terms of mononomials, also using a graphical technique. It was going to be used for a first-principles method of evaluating plethysms but was not used.

4. OTHER SPECIAL PROGRAMMES

The only problem remaining other than straightforward techniques of combining the above operations, is the operations of plethysm. PLETH2 calculates simply and directly $\{m\} \otimes \{n\}$ where $\{m\}$ is an S-function on two variables. This is required in calculating branching rules from higher groups to R_3. $\{m\} \otimes \{n\}$ on an unrestricted number of variables is quite easily done by Murnaghan's method. PLIC calculates by this method using PLI to give it known results. This it does by calculation if m or n are less than or equal to two, or by requesting PLNUM to look up a table. PLNUM is also used to store results in this table. The general (outer) plethysm programme (PLETH) uses PLHL, PLIL and PLI to calculate any plethysm by using the S-functions separated (by SPLIT) into sums of products of completely symmetric parts (h_r's).

As suggested in the section on inner plethysms, a similar method could be used for this problem, the most difficult step being to write an S-function as an inner product of S-functions of the form $\{m-k,1^k\}$.

A routine PCHMOD is used when generating the table of $\{m\} \otimes \{n\}$ to punch a module deck of the table in a form suitable for linkage editing into the other plethysm jobs. This method is more convenient than reading the data in off cards.

5. PHASE OVERLAY

The University of Canterbury's IBM 360/44 had a core storage size of 16 K bytes until mid 1969 when it was increased to 32 K. The programmes, without the working matrices more than filled this smaller size and were used with phase overlay to give the required space for the working areas. So-called "root-phase overlay" was used, whereby the main programme is premanently resident in core. Three phases will then read alternately into the 8K remaining. These phases were:

a) The header phase, including DUDLEY, HEADER and IBCOM.

b) The algebra phase, including all the calculation routines.

c) The output phase.

DUDLEY thus was made to consist of two control sections, one ov which was permanently resident to make full use of the multibuffering. The FORTRAN phase overlay routines are not suitable for use when IBCOM is being overlayed and two assembler routines were used. OVER performs the overlaying and INIBC initializes or de-initializes IBCOM each time it is read in or out. (This is only when HEADER is used).

With the larger core size now available no programme requires overlay except that an inner plethysm programme would require more storage if any but relatively trivial examples were to be calculated.

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APPENDIX I

CORRIGENDA TO

"The Theory of Group Characters", D.E. Littlewood[7]

p.238: In giving eqs (11.9;1) to (11.9;6) it would be desirable to omit the identity (1) appearing on the right-hand-side as it is already incorporated in the series given below. Perhaps (11.9;5) and (11.9;6) could be better written as

$$\Pi(1-\theta\alpha_i)\ \Pi(1-\alpha_i\alpha_j) \quad = \quad \Sigma\ \theta^p(-1)^{\frac{1}{2}(p+r)}\{\varepsilon\} \qquad (11.9;5)$$

and

$$1/\Pi(1-\theta\alpha_i)\ \Pi(1-\alpha_i\alpha_j) \quad = \quad \Sigma\ \theta^p\ \{\zeta\} \qquad (11.9;6)$$

where $\theta = \pm 1$.

p.243: Theorem V

$$[\lambda] \quad = \quad \Sigma\ (-1)^{\frac{1}{2}(p+r)}\ (-\theta)^p\ g_{\varepsilon\eta\lambda}\{\eta\}'.$$

p.247: II. ... those S-functions $\{\alpha\}$ defined by (11.9;1) ... 5 lines from bottom, and bottom line replace Δ by Δ^2.

p.248: Line 3. Replace 2^ν by $2^{2\nu}$.

p.255: 4 lines from bottom replace ϕ_r by $\frac{1}{2}\phi_r$ - twice.

p.257: Replace Δ by Δ^2 five times

Line 16 $n = 2\nu+1$.

p.256: It would be worthwhile giving the result

$$[(\tfrac{1}{2})^\nu]\{\lambda\} = \Sigma g_{\zeta\eta\lambda}[\eta_1+\tfrac{1}{2},\eta_2+\tfrac{1}{2},\cdots,\eta_\nu+\tfrac{1}{2}].$$

p.259: I obtain IX as

$$[\lambda_1+\tfrac{1}{2},\lambda_2+\tfrac{1}{2},\cdots,\lambda_\nu+\tfrac{1}{2}] = \Pi(2_i \sin \tfrac{1}{2}\phi_r)[\Sigma(-1)^{\frac{1}{2}(p-r)} g_{\varepsilon\eta\lambda}\{\eta\}]$$

$$= (i)^\nu \frac{|S_t^{\lambda_s+\nu-s+\frac{1}{2}}|}{|C_t^{(\nu-s)}|} .$$

The inverse relation

$$\Pi(2_i \sin \tfrac{1}{2}\phi_r)\{\lambda\} = \Sigma(-1)^p\, g_{\zeta\eta\lambda}[\eta_1+\tfrac{1}{2},\eta_2+\tfrac{1}{2},\cdots,\eta_\nu+\tfrac{1}{2}]$$

then follows.

p.294: 6 lines from bottom replace

$$\{r+\lambda_1,r+\lambda_2,\cdots r+\lambda_\nu,r-\mu_\nu,\cdots,\nu-\mu_1\}$$

by

$$\{r+\lambda_1,r+\lambda_2,\cdots,r+\lambda_\nu,r-\mu_\nu,\cdots,r-\mu_1\}.$$

APPENDIX II

HYDROGEN RADIAL INTEGRALS

Following Messiah[73] we write a hydrogenic eigenfunction as:

$$\psi_{n\ell m}(r\theta\phi) = R_{n\ell}(r)\; Y_\ell^m(\theta,\phi) \tag{A.1}$$

$$R_{n\ell}(r) = a^{-\frac{3}{2}}\; N_{n\ell}\; F_{n\ell}\left(\frac{2r}{na}\right) \tag{A.2}$$

where Y_ℓ^m are the usual normalized spherical harmonics, $F_{n\ell}$ is the Laguerre polynomial, given for example, by Bateman[74], and a is related to the radius of a Bohr orbit.

$$a = \frac{h^2}{Zm'e^2} \tag{A.3}$$

$$N_{n\ell} = \frac{2}{n^2} \left| \frac{(n-\ell-1)!}{(n+\ell)!} \right|^{\frac{1}{2}} \tag{A.4}$$

$$F_{n\ell}(x) = x^\ell\; e^{-\frac{1}{2}x}\; L_{n-\ell-1}^{2\ell+1}(x). \tag{A.5}$$

$L_p^k(x)$ is related to the confluent hypergeometric series $F(\alpha|\beta|x)$

$$L_p^k(x) = \frac{(p+k)!}{p!k!}\; F\,(-p|k+1|x) \tag{A.6}$$

$$= \sum_{s=0}^{p} (-1)^s \frac{(p+k)!}{(p-s)!(k+s)!s!}\; x^s \tag{A.7}$$

Substitution of these radial functions into the radial integral of Condon and Shortley:

$$R^k(n_a\ell_a,n_b\ell_b;n_c\ell_c,n_d\ell_d) \equiv R^k(AB;CD)$$

$$= \int_0^\infty \int_0^\infty \frac{r_<^{\,k}}{r_>^{\,k+1}} R_A(r_i)R_B(r_j)R_C(r_i)R_D(r_j)\; r_i^{\,2} r_j^{\,2}\; dr_i dr_j \tag{A.8}$$

$$= \int_0^\infty R_A(r_i)R_C(r_i)r_i^{-k+1}\int_0^{r_i} r_j^{k+2}\; R_B(r_j)R_D(r_j)\; dr_j dr_i$$

$$+ \int_0^\infty R_B(r_j)R_D(r_j)\; r_j^{-k+1} \int_0^{r_j} r_i^{k+2}\; R_A(r_i)R_C(r_i)\, dr_i dr_j \tag{A.9}$$

leads to integrals of the form

$$J(a,b) = \int_0^\infty \rho^a\, e^{-\rho} \int_0^\rho \sigma^b e^{-\sigma}\; d\sigma\; d\rho \tag{A.10}$$

Judd[27] shows that

$$J(a,b) = a!b! - b! \sum_{r=0}^{b} \frac{(a+r)!}{r!\,2^{a+r+1}} \tag{A.11}$$

$$= \frac{(a+b+1)!}{(b+1)\,2^{a+b+2}}\; F(a+b+2,1;b+2;\tfrac{1}{2}) \tag{A.12}$$

Values of this hypergeometric function may be found using,

$$F(u,1;u;\tfrac{1}{2}) = 2 \tag{A.13}$$

and the recurrence relations:

$$xF(x+1,1;u;\tfrac{1}{2}) = 2(u-1) + 2(x-u+1)\, F\, (x,1;u;\tfrac{1}{2})$$
$$yF(u,1;y;\tfrac{1}{2}) = 2y + (u-y)\, F\, (u,1;y+1;\tfrac{1}{2}) \qquad \text{(A.14)}$$

Thus we have

$$F^0(1s,1s) = \frac{1}{a} \cdot \frac{5}{8} \qquad F^0(1s,2p) = \frac{1}{a} \cdot \frac{7.11}{3^5}$$

$$F^0(2s,2s) = \frac{1}{a} \cdot \frac{7.11}{2^9} \qquad F^0(2s,2p) = \frac{1}{a} \cdot \frac{13^2}{2^{10}}$$

$$F^0(2p,2p) = \frac{1}{a} \cdot \frac{3.31}{2^9} \qquad G^0(1s,2p) = \frac{1}{a} \cdot \frac{2^4}{3^6}$$

$$F^2(2p,2p) = \frac{1}{a} \cdot \frac{3.3.5}{2^9} \qquad G^1(1s,2p) = \frac{1}{a} \cdot \frac{2^4.7}{3^7}$$

$$F^0(1s,2s) = \frac{1}{a} \cdot \frac{7}{3^3} \qquad G^1(2s,2p) = \frac{1}{a} \cdot \frac{3^2.5}{2^9}$$

APPENDIX III

TABLES OF GROUP AND S-FUNCTION PROPERTIES

In the following pages we present several tables of group and S-function properties.

The tables of branching rules required for the $(s+p+d)^N$ electronic configuration were calculated by hand using the methods in the text. Both tables require the use of plethysm and could now be machine computed.

The other tables were machine computed and checked and have been reproduced photographically to eliminate copying errors. Two special notations are used however:

1) When writing a spin representation of R_8

$$[\lambda] \equiv \left[\frac{\mu_1}{2}, \frac{\mu_2}{2}, \cdots\right] \qquad (\mu_i \text{ odd})$$

we have written $[\mu]'$ since the computer could not write fractions.

2) For the table of plethysms of one part we have listed $\{m\} \otimes \{n\}$ and $\{m\} \otimes \{1^n\}$ for $mn \leq 22$. The latter we have written $\{n\}'$ which is to be interpreted as $\{\tilde{n}\} \equiv \{1^n\}$.

Decompositions of Irreducible Representations for

$Sp_{18} \rightarrow SU_2 \times R_9$

$f^{\langle\lambda\rangle}$	Sp_{18}	$SU_2 \times R_9$
1	0	$^{1}[0000]$
18	1	$^{2}[1000]$
152	2	$^{3}[1100]\,^{1}[2000]$
798	3	$^{4}[1110]\,^{2}[2100]$
2907	4	$^{5}[1111]\,^{3}[2110]\,^{1}[2200]$
7752	5	$^{6}[1111]\,^{4}[2111]\,^{2}[2210]$
15504	6	$^{7}[1110]\,^{5}[2111]\,^{3}[2211]\,^{1}[2220]$
23256	7	$^{8}[1100]\,^{6}[2110]\,^{4}[2211]\,^{2}[2221]$
25194	8	$^{9}[1000]\,^{7}[2100]\,^{5}[2210]\,^{3}[2221]\,^{1}[2222]$
16796	9	$^{10}[0000]\,^{8}[2000]\,^{6}[2200]\,^{4}[2220]\,^{2}[2222]$

Decompositions of Irreducible Representations for $R_9 \to R_4$

$f^{[\lambda]}$	R_9	O_4
1	[0000]	[00]
9	[1000]	[20]
36	[1100]	[31][11]
84	[1110]	[40][33][31][20][11]
126	[1111]	$[42][40][31][22][20]^2[00]$
44	[2000]	[40][22][20]
231	[2100]	$[51][42][40][31]^2[22][20]^2[11]$
594	[2110]	$[60][53][51]^2[42]^2[40]^3[33][31]^4[22][20]^4[11]^2$
924	[2111]	$[62][60][53][51]^3[44][42]^3[40]^5[33][31]^5[22]^3[20]^5[11]^2[00]$
495	[2200]	$[62][60][51][44][42]^2[40]^3[31]^2[22]^2[20]^3[00]^2$
1650	[2210]	$[71][64][62]^2[60]^3[53]^2[51]^4[44][42]^5[40]^8[33]^2[31]^6[22]^3[20]^7[11]^2[00]^2$
2772	[2211]	$[73][71]^2[64][62]^3[60]^4[55][53]^4[51]^8[44][42]^7[40]^{10}[33]^4[31]^{11}[22]^3[20]^8[11]^5$
1980	[2220]	$[80][73][71][66][64][62]^3[60]^4[53]^2[51]^4[44]^2[42]^5[40]^8[33]^2[31]^5[22]^3[20]^6[11][00]^3$
4158	[2221]	$[82][80][75][73]^2[71]^3[64]^2[62]^5[60]^7[55][53]^6[51]^{10}[44]^2[42]^9[40]^{12}[33]^4[31]^{12}[22]^4[20]^9[11]^4[00]$
2772	[2222]	$[84][82][80][73][71]^2[64]^2[62]^4[60]^4[55][53]^3[51]^6[44]^2[42]^6[40]^8[33][31]^5[22]^4[20]^6[11][00]$

<u>Kronecker Products of Spin Representations of R_8</u>

[1111]' x [1111]' = [0000] + [1100] + [1111]
[111-1]' x [1111]' = [1000] + [1110]
[111-1]' x [111-1]' = [0000] + [1100] + [111-1]

[3111]' x [1111]' = [1000] + [1110] + [2100] + [2111]
[3111]' x [111-1]' = [1100] + [1111] + [2000] + [2110]
[3111]' x [3111]' = [0000] +2[1100] + [111-1] + [1111] + [2000] +2[2110] + [2200] + [2211]
+ [3100] + [3111]
[311-1]' x [1111]' = [1100] + [111-1] + [2000] + [2110]
[311-1]' x [111-1]' = [1000] + [1110] + [2100] + [211-1]
[311-1]' x [3111]' = [1000] +2[1110] +2[2100] + [211-1] + [2111] + [2210] + [3000]
+ [3110]
[311-1]' x [311-1]' = [0000] +2[1100] + [111-1] + [1111] + [2000] +2[2110] + [2200]
+ [221-1] + [3100] + [311-1]
[3311]' x [1111]' = [1100] + [1111] + [2110] + [2200] + [2211]
[3311]' x [111-1]' = [1110] + [2100] + [2111] + [2210]
[3311]' x [3111]' = [1000] +2[1110] +2[2100] + [211-1] +2[2111] +2[2210] + [2221] + [3110]
+ [3200] + [3211]
[3311]' x [311-1]' = [1100] + [111-1] + [1111] + [2000] +3[2110] + [2200] + [221-1]
+ [2211] + [2220] + [3100] + [3111] + [3210]
[3311]' x [3311]' = [0000] +2[1100] + [111-1] +2[1111] + [2000] +3[2110] +2[2200]
+ [221-1] +3[2211] + [2220] + [2222] + [3100] + [311-1] + [3111] +2[3210]
+ [3221] + [3300] + [3311]
[331-1]' x [1111]' = [1110] + [2100] + [211-1] + [2210]
[331-1]' x [111-1]' = [1100] + [111-1] + [2110] + [2200] + [221-1]
[331-1]' x [3111]' = [1100] + [111-1] + [1111] + [2000] +3[2110] + [2200] + [221-1]
+ [2211] + [2220] + [3100] + [311-1] + [3210]
[331-1]' x [311-1]' = [1000] +2[1110] +2[2100] +2[211-1] + [2111] +2[2210] + [222-1]
+ [3110] + [3200] + [321-1]
[331-1]' x [3311]' = [1000] +2[1110] +2[2100] +2[211-1] +2[2111] +3[2210] + [222-1]
+ [2221] + [3000] +2[3110] + [3200] + [321-1] + [3211] + [3220] + [3310]
[331-1]' x [331-1]' = [0000] +2[1100] +2[111-1] + [1111] + [2000] +3[2110] +2[2200]
+3[221-1] + [2211] + [222-2] + [2220] + [3100] + [311-1] + [3111]
+2[3210] + [322-1] + [3300] + [331-1]
[3331]' x [1111]' = [1110] + [2111] + [2210] + [2221]
[3331]' x [111-1]' = [1111] + [2110] + [2211] + [2220]
[3331]' x [3111]' = [1100] + [111-1] + [1111] +2[2110] + [2200] + [221-1] +2[2211]
+ [2220] + [2222] + [3111] + [3210] + [3221]
[3331]' x [311-1]' = [1110] + [2100] + [211-1] +2[2111] +2[2210] + [222-1] + [2221]
+ [3110] + [3211] + [3220]
[3331]' x [3311]' = [1000] +2[1110] +2[2100] + [211-1] +2[2111] +3[2210] +2[2221] + [3110]
+ [3200] + [321-1] +2[3211] + [3220] + [3222] + [3310] + [3321]
[3331]' x [331-1]' = [1100] + [1111] + [2000] +3[2110] + [2200] + [221-1] +2[2211]
+2[2220] + [3100] + [311-1] + [3111] +2[3210] + [322-1] + [3221]
+ [3311] + [3320]
[3331]' x [3331]' = [0000] +2[1100] + [111-1] + [1111] + [2000] +2[2110] +2[2200]
+ [221-1] +2[2211] + [2220] + [2222] + [3100] + [3111] +2[3210] +2[3221]
+ [3300] + [331-1] + [3311] + [3320] + [3322] + [3331]
[333-1]' x [1111]' = [111-1] + [2110] + [221-1] + [2220]
[333-1]' x [111-1]' = [1110] + [211-1] + [2210] + [222-1]
[333-1]' x [3111]' = [1110] + [2100] +2[211-1] + [2111] +2[2210] + [222-1] + [2221]
+ [3110] + [321-1] + [3220]
[333-1]' x [311-1]' = [1100] + [111-1] + [1111] +2[2110] + [2200] +2[221-1] + [2211]
+ [222-2] + [2220] + [311-1] + [3210] + [322-1]
[333-1]' x [3311]' = [1100] + [111-1] + [2000] +3[2110] + [2200] +2[221-1] + [2211]
+2[2220] + [3100] + [311-1] + [3111] +2[3210] + [322-1] + [3221]
+ [331-1] + [3320]
[333-1]' x [331-1]' = [1000] +2[1110] +2[2100] +2[211-1] + [2111] +3[2210] +2[222-1]
+ [3110] + [3200] +2[321-1] + [3211] + [322-2] + [3220] + [3310]
+ [332-1]
[333-1]' x [3331]' = [1000] + [1110] +2[2100] + [211-1] + [2111] +2[2210] + [222-1]
+ [2221] + [3000] +2[3110] + [3200] + [321-1] + [3211] +2[3220] + [3310]
+ [332-1] + [3321] + [3330]
[333-1]' x [333-1]' = [0000] +2[1100] + [111-1] + [1111] + [2000] +2[2110] +2[2200]
+2[221-1] + [2211] + [222-2] + [2220] + [3100] + [311-1] +2[3210]
+2[322-1] + [3300] + [331-1] + [3311] + [332-2] + [3320] + [333-1]
[3333]' x [1111]' = [1111] + [2211] + [2222]
[3333]' x [111-1]' = [2111] + [2221]
[3333]' x [3111]' = [1110] + [2111] + [2210] + [2221] + [3211] + [3222]
[3333]' x [311-1]' = [2110] + [2211] + [2220] + [3111] + [3221]

Kronecker Products of Spin Representations of R_8 (contd)

[3333]' x [3311]' = [1100] + [1111] + [2110] + [2200] +2[2211] + [2222] + [3210] + [3221]
+ [3311] + [3322]

[3333]' x [331-1]' = [2100] + [2111] + [2210] + [2221] + [3110] + [3211] + [3220] + [3321]

[3333]' x [3331]' = [1000] + [1110] + [2100] + [2111] + [2210] + [2221] + [3200] + [3211]
+ [3222] + [3310] + [3321] + [3332]

[3333]' x [333-1]' = [2000] + [2110] + [2220] + [3100] + [3111] + [3210] + [3221] + [3320]
+ [3331]

[3333]' x [3333]' = [0000] + [1100] + [1111] + [2200] + [2211] + [2222] + [3300] + [3311]
+ [3322] + [3333]

[333-3]' x [1111]' = [211-1] + [222-1]

[333-3]' x [111-1]' = [111-1] + [221-1] + [222-2]

[333-3]' x [3111]' = [2110] + [221-1] + [2220] + [311-1] + [322-1]

[333-3]' x [311-1]' = [1110] + [211-1] + [2210] + [222-1] + [321-1] + [322-2]

[333-3]' x [3311]' = [2100] + [211-1] + [2210] + [222-1] + [3110] + [321-1] + [3220]
+ [332-1]

[333-3]' x [331-1]' = [1100] + [111-1] + [2110] + [2200] +2[221-1] + [222-2] + [3210]
+ [322-1] + [331-1] + [332-2]

[333-3]' x [3331]' = [2000] + [2110] + [2220] + [3100] + [311-1] + [3210] + [322-1]
+ [3320] + [333-1]

[333-3]' x [333-1]' = [1000] + [1110] + [2100] + [211-1] + [2210] + [222-1] + [3200]
+ [321-1] + [322-2] + [3310] + [332-1] + [333-2]

[333-3]' x [3333]' = [3000] + [3110] + [3220] + [3330]

[333-3]' x [333-3]' = [0000] + [1100] + [111-1] + [2200] + [221-1] + [222-2] + [3300]
+ [331-1] + [332-2] + [333-3]

The Expansion of S-Functions as Mononomials

{0} = (0)

{1} = (1)

{2} = (11) + (2)
{11} = (11)

{3} = (111) + (21) + (3)
{21} =2(111) + (21)
{111} = (111)

{4} = (1111) + (211) + (22) + (31) + (4)
{31} =3(1111) +2(211) + (22) + (31)
{22} =2(1111) + (211) + (22)
{211} =3(1111) + (211)
{1111} = (1111)

{5} = (11111) + (2111) + (221) + (311) + (32) + (41) + (5)
{41} =4(11111) +3(2111) +2(221) +2(311) + (32) + (41)
{32} =5(11111) +3(2111) +2(221) + (311) + (32)
{311} =6(11111) +3(2111) + (221) + (311)
{221} =5(11111) + (2111) + (221)
{2111} =4(11111) + (2111)
{11111} = (11111)

{6} = (111111) + (21111) + (2211) + (222) + (3111) + (321) + (33) + (411) + (42) + (51)
+ (6)
{51} =5(111111) +4(21111) +3(2211) +2(222) +3(3111) +2(321) + (33) +2(411) + (42) + (51)
{42} =9(111111) +6(21111) +4(2211) +3(222) +3(3111) +2(321) + (33) + (411) + (42)
{411} =10(111111) +6(21111) +3(2211) +2(222) +3(3111) + (321) + (33) + (411)
{33} =5(111111) +3(21111) +2(2211) + (222) + (3111) + (321) + (33)
{321} =16(111111) +8(21111) +4(2211) +2(222) + (3111) + (321)
{3111} =10(111111) +4(21111) + (2211) + (222) + (3111)
{222} =5(111111) + (21111) + (2211) + (222)
{2211} =9(111111) + (21111) + (2211)
{21111} =5(111111) + (21111)
{111111} = (111111)

{7} = (1111111) + (211111) + (22111) + (2221) + (31111) + (3211) + (322) + (331) + (4111)
+ (421) + (43) + (511) + (52) + (61) + (7)
{61} =6(1111111) +5(211111) +4(22111) +3(2221) +4(31111) +3(3211) +2(322) +2(331) +3(4111)
+2(421) + (43) +2(511) + (52) + (61)
{52} =14(1111111) +10(211111) +7(22111) +5(2221) +6(31111) +4(3211) +3(322) +2(331)
+3(4111) +2(421) + (43) + (511) + (52)
{511} =15(1111111) +10(211111) +6(22111) +3(2221) +6(31111) +3(3211) +2(322) + (331)
+3(4111) + (421) + (43) + (511)
{43} =14(1111111) +9(211111) +6(22111) +4(2221) +4(31111) +3(3211) +2(322) +2(331)
+ (4111) + (421) + (43)
{421} =35(1111111) +20(211111) +11(22111) +6(2221) +8(31111) +4(3211) +2(322) + (331)
+ (4111) + (421)
{4111} =20(1111111) +10(211111) +4(22111) +2(2221) +4(31111) + (3211) + (322) + (331)
+ (4111)
{331} =21(1111111) +11(211111) +6(22111) +3(2221) + (31111) + (3211) + (322) + (331)
{322} =21(1111111) +10(211111) +5(22111) +3(2221) + (31111) + (3211) + (322)
{3211} =35(1111111) +15(211111) +6(22111) +2(2221) + (31111) + (3211)
{31111} =15(1111111) +5(211111) + (22111) + (2221) + (31111)
{2221} =14(1111111) +2(211111) + (22111) + (2221)
{22111} =14(1111111) + (211111) + (22111)
{211111} =6(1111111) + (211111)
{1111111} = (1111111)

{8} = (11111111) + (2111111) + (221111) + (22211) + (2222) + (311111) + (32111) + (3221)
+ (3311) + (332) + (41111) + (4211) + (422) + (431) + (44) + (5111) + (521) + (53)
+ (611) + (62) + (71) + (8)
{71} =7(11111111) +6(2111111) +5(221111) +4(22211) +3(2222) +5(311111) +4(32111) +3(3221)
+3(3311) +2(332) +4(41111) +3(4211) +2(422) +2(431) + (44) +3(5111) +2(521) + (53)
+2(611) + (62) + (71)
{62} =20(11111111) +15(2111111) +11(221111) +8(22211) +6(2222) +10(311111) +7(32111)
+5(3221) +4(3311) +3(332) +6(41111) +4(4211) +3(422) +2(431) + (44) +3(5111) +2(521)
+ (53) + (611) + (62)

The Expansion of S-Functions as Mononomials (contd)

{611} =21(11111111) +15(2111111) +10(221111) +6(22211) +4(2222) +10(311111) +6(32111)
+3(3221) +3(3311) +2(332) +6(41111) +3(4211) +2(422) + (431) + (44) +3(5111) + (521)
+ (53) + (611)

{53} =28(11111111) +19(2111111) +13(221111) +9(22211) +6(2222) +10(311111) +7(32111)
+5(3221) +4(3311) +3(332) +4(41111) +3(4211) +2(422) +2(431) + (44) + (5111) + (521)
+ (53)

{521} =64(11111111) +40(2111111) +24(221111) +14(22211) +8(2222) +20(311111) +11(32111)
+6(3221) +4(3311) +2(332) +8(41111) +4(4211) +2(422) + (431) + (44) + (5111) + (521)

{5111} =35(11111111) +20(2111111) +10(221111) +4(22211) +2(2222) +10(311111) +4(32111)
+2(3221) + (3311) + (332) +4(41111) + (4211) + (422) + (431) + (44) + (5111)

{44} =14(11111111) +9(2111111) +6(221111) +4(22211) +3(2222) +4(311111) +3(32111) +2(3221)
+2(3311) + (332) + (41111) + (4211) + (422) + (431) + (44)

{431} =70(11111111) +40(2111111) +23(221111) +13(22211) +7(2222) +15(311111) +9(32111)
+5(3221) +4(3311) +2(332) + (41111) + (4211) + (422) + (431)

{422} =56(11111111) +30(2111111) +16(221111) +9(22211) +6(2222) +10(311111) +5(32111)
+3(3221) + (3311) + (332) + (41111) + (4211) + (422)

{4211} =90(11111111) +45(2111111) +21(221111) +9(22211) +4(2222) +15(311111) +6(32111)
+2(3221) + (3311) + (332) + (41111) + (4211)

{41111} =35(11111111) +15(2111111) +5(221111) +2(22211) + (2222) +5(311111) + (32111)
+ (3221) + (3311) + (332) + (41111)

{332} =42(11111111) +21(2111111) +11(221111) +6(22211) +3(2222) + (311111) + (32111)
+ (3221) + (3311) + (332)

{3311} =56(11111111) +26(2111111) +12(221111) +5(22211) +3(2222) + (311111) + (32111)
+ (3221) + (3311)

{3221} =70(11111111) +30(2111111) +13(221111) +6(22211) +3(2222) +2(311111) + (32111)
+ (3221)

{32111} =64(11111111) +24(2111111) +8(221111) +2(22211) + (2222) + (311111) + (32111)

{311111} =21(11111111) +6(2111111) + (221111) + (22211) + (2222) + (311111)

{2222} =14(11111111) +2(2111111) + (221111) + (22211) + (2222)

{22211} =28(11111111) +3(2111111) + (221111) + (22211)

{221111} =20(11111111) + (2111111) + (221111)

{2111111} =7(11111111) + (2111111)

{11111111} = (11111111)

<u>The Outer Plethysm of S-Functions of One Part</u>

$\{2\} \otimes \{2\} = \{22\} + \{4\}$
$\{2\} \otimes \{2\}' = \{31\}$

$\{3\} \otimes \{2\} = \{42\} + \{6\}$
$\{3\} \otimes \{2\}' = \{33\} + \{51\}$
$\{2\} \otimes \{3\} = \{222\} + \{42\} + \{6\}$
$\{2\} \otimes \{3\}' = \{33\} + \{411\}$

$\{4\} \otimes \{2\} = \{44\} + \{62\} + \{8\}$
$\{4\} \otimes \{2\}' = \{53\} + \{71\}$
$\{2\} \otimes \{4\} = \{2222\} + \{422\} + \{44\} + \{62\} + \{8\}$
$\{2\} \otimes \{4\}' = \{431\} + \{5111\}$

$\{3\} \otimes \{3\} = \{441\} + \{522\} + \{63\} + \{72\} + \{9\}$
$\{3\} \otimes \{3\}' = \{333\} + \{531\} + \{63\} + \{711\}$

$\{5\} \otimes \{2\} = \{64\} + \{82\} + \{10\}$
$\{5\} \otimes \{2\}' = \{55\} + \{73\} + \{91\}$
$\{2\} \otimes \{5\} = \{22222\} + \{4222\} + \{442\} + \{622\} + \{64\} + \{82\} + \{10\}$
$\{2\} \otimes \{5\}' = \{442\} + \{5311\} + \{61111\}$

$\{6\} \otimes \{2\} = \{66\} + \{84\} + \{102\} + \{12\}$
$\{6\} \otimes \{2\}' = \{75\} + \{93\} + \{111\}$
$\{4\} \otimes \{3\} = \{444\} + \{642\} + \{66\} + \{741\} + \{822\} + \{84\} + \{93\} + \{102\} + \{12\}$
$\{4\} \otimes \{3\}' = \{552\} + \{633\} + \{741\} + \{75\} + \{831\} + \{93\} + \{1011\}$
$\{3\} \otimes \{4\} = \{444\} + \{5421\} + \{6222\} + \{642\} + \{66\} + \{732\} + \{741\} + \{822\} + \{84\} + \{93\}$
$+ \{102\} + \{12\}$
$\{3\} \otimes \{4\}' = \{3333\} + \{5331\} + \{5511\} + \{633\} + \{642\} + \{66\} + \{7311\} + \{741\} + \{831\}$
$+ \{9111\}$
$\{2\} \otimes \{6\} = \{222222\} + \{42222\} + \{4422\} + \{444\} + \{6222\} + \{642\} + \{66\} + \{822\} + \{84\}$
$+ \{102\} + \{12\}$
$\{2\} \otimes \{6\}' = \{444\} + \{5421\} + \{63111\} + \{711111\}$

$\{7\} \otimes \{2\} = \{86\} + \{104\} + \{122\} + \{14\}$
$\{7\} \otimes \{2\}' = \{77\} + \{95\} + \{113\} + \{131\}$
$\{2\} \otimes \{7\} = \{2222222\} + \{422222\} + \{44222\} + \{4442\} + \{62222\} + \{6422\} + \{644\} + \{662\}$
$+ \{8222\} + \{842\} + \{86\} + \{1022\} + \{104\} + \{122\} + \{14\}$
$\{2\} \otimes \{7\}' = \{5441\} + \{5522\} + \{64211\} + \{731111\} + \{8111111\}$

$\{5\} \otimes \{3\} = \{663\} + \{744\} + \{852\} + \{861\} + \{942\} + \{96\} + \{1041\} + \{105\} + \{1122\} + \{114\}$
$+ \{123\} + \{132\} + \{15\}$
$\{5\} \otimes \{3\}' = \{555\} + \{753\} + \{771\} + \{852\} + \{933\} + \{951\} + \{96\} + \{1041\} + \{105\}$
$+ \{1131\} + \{123\} + \{1311\}$
$\{3\} \otimes \{5\} = \{5442\} + \{55311\} + \{64221\} + \{6441\} + \{6522\} + \{663\} + \{72222\} + \{7422\}$
$+ \{7431\} + \{744\} + \{7521\} + \{762\} + \{8322\} + \{8421\} + \{843\} + \{852\} + \{861\}$
$+ \{9222\} + 2\{942\} + \{96\} + \{1032\} + \{1041\} + \{105\} + \{1122\} + \{114\} + \{123\}$
$+ \{132\} + \{15\}$
$\{3\} \otimes \{5\}' = \{33333\} + \{53331\} + \{55311\} + \{6333\} + \{6432\} + \{6531\} + \{663\} + \{73311\}$
$+ \{7431\} + \{744\} + \{75111\} + \{7521\} + \{762\} + \{8331\} + \{8421\} + \{843\} + \{8511\}$
$+ \{861\} + \{93111\} + \{9411\} + \{942\} + \{10311\} + \{111111\}$

$\{8\} \otimes \{2\} = \{88\} + \{106\} + \{124\} + \{142\} + \{16\}$
$\{8\} \otimes \{2\}' = \{97\} + \{115\} + \{133\} + \{151\}$
$\{4\} \otimes \{4\} = \{4444\} + \{6442\} + \{6622\} + \{664\} + \{7441\} + \{7531\} + \{763\} + \{7711\} + \{8422\}$
$+2\{844\} + \{8521\} +2\{862\} + \{88\} + \{9421\} + \{943\} + \{952\} + \{961\} + \{10222\}$
$+2\{1042\} + \{1051\} +2\{106\} + \{1132\} + \{1141\} + \{1222\} +2\{124\} + \{133\} + \{142\}$
$+ \{16\}$
$\{4\} \otimes \{4\}' = \{5551\} + \{6532\} + \{7333\} + \{7531\} + \{754\} + \{763\} + \{7711\} + \{8431\} + \{8521\}$
$+ \{853\} + \{862\} + \{871\} + \{9331\} + \{943\} + \{9511\} + \{952\} + \{961\} + \{1033\}$
$+ \{10411\} + \{1042\} + \{1051\} + \{106\} + \{11311\} + \{1141\} + \{1231\} + \{13111\}$
$\{2\} \otimes \{8\} = \{22222222\} + \{4222222\} + \{442222\} + \{44422\} + \{4444\} + \{622222\} + \{64222\}$
$+ \{6442\} + \{6622\} + \{664\} + \{82222\} + \{8422\} + \{844\} + \{862\} + \{88\} + \{10222\}$
$+ \{1042\} + \{106\} + \{1222\} + \{124\} + \{142\} + \{16\}$
$\{2\} \otimes \{8\}' = \{5542\} + \{64411\} + \{65221\} + \{742111\} + \{8311111\} + \{91111111\}$

$\{9\} \otimes \{2\} = \{108\} + \{126\} + \{144\} + \{162\} + \{18\}$
$\{9\} \otimes \{2\}' = \{99\} + \{117\} + \{135\} + \{153\} + \{171\}$
$\{6\} \otimes \{3\} = \{666\} + \{864\} + \{882\} + \{963\} + \{1044\} + \{1062\} + \{1071\} + \{108\} + \{1152\}$
$+ \{1161\} + \{1242\} +2\{126\} + \{1341\} + \{135\} + \{1422\} + \{144\} + \{153\} + \{162\}$
$+ \{18\}$

The Outer Plethysm of S-Functions of One Part (contd)

{6} ⊗ {3}' = {774} + {855} + {963} + {972} + {99} + {1053} + {1071} + {1152} + {1161}
+ {117} + {1233} + {1251} + {126} + {1341} + {135} + {1431} + {153} + {1611}

{3} ⊗ {6} = {55431} + {555111} + {64422} + {6444} + {653211} + {65421} + {66222} + {6642}
+ {666} + {742221} + {74421} + {7443} + {75222} + {75321} + {75411} + {7542}
+ {76221} + {7632} + {7641} + {7731} + {822222} + {84222} + {84321} +2{8442}
+ {85221} + {85311} + {8532} + {8541} +2{8622} + {8631} +2{864} + {8721} + {882}
+ {93222} + {94221} + {9432} +2{9441} +2{9522} + {9531} + {9621} +2{963} + {972}
+ {102222} +2{10422} + {10431} +2{1044} + {10521} + {1053} +2{1062} + {1071}
+ {108} + {11322} + {11421} + {1143} +2{1152} + {1161} + {12222} +2{1242}
+2{126} + {1332} + {1341} + {135} + {1422} + {144} + {153} + {162} + {18}

{3} ⊗ {6}' = {333333} + {533331} + {553311} + {555111} + {63333} + {64332} + {65331}
+ {65421} +2{6633} + {6651} + {733311} + {74331} + {7443} + {753111} + {75321}
+ {75411} + {7542} + {76311} + {7632} + {7641} + {771111} + {7722} + {774}
+ {83331} + {84321} + {8433} + {8442} +2{85311} + {8532} + {8541} + {86211}
+2{8631} + {864} + {8721} + {8811} + {933111} + {94311} + {9432} +2{9441}
+ {951111} + {95211} + {9522} + {9531} + {96111} + {9621} + {963} + {972}
+ {103311} + {104211} + {10431} + {1044} + {105111} + {10521} + {10611}
+ {1131111} + {114111} + {11421} + {123111} + {1311111}

{2} ⊗ {9} = {222222222} + {42222222} + {4422222} + {444222} + {44442} + {6222222}
+ {642222} + {64422} + {6444} + {66222} + {6642} + {666} + {822222} + {84222}
+ {8442} + {8622} + {864} + {882} + {102222} + {10422} + {1044} + {1062} + {108}
+ {12222} + {1242} + {126} + {1422} + {144} + {162} + {18}

{2} ⊗ {9}' = {5553} + {65421} + {66222} + {744111} + {752211} + {8421111} + {93111111}
+ {1011111111}

{10} ⊗ {2} = {1010} + {128} + {146} + {164} + {182} + {20}

{10} ⊗ {2}' = {119} + {137} + {155} + {173} + {191}

{5} ⊗ {4} = {6662} + {7643} + {8444} + {8642} + {8651} + {866} + {8741} + {8822} + {884}
+ {9542} + {9632} + {9641} + {965} + {9731} + {974} + {9821} + {983} + {10442}
+ {10541} + {10622} + {10631} +3{1064} + {10721} + {1073} +2{1082} + {1091}
+ {1010} + {11441} + {11522} + {11531} + {1154} + {11621} +2{1163} + {11711}
+2{1172} + {1181} + {12422} +2{1244} + {12521} + {1253} +3{1262} + {1271}
+2{128} + {13421} + {1343} +2{1352} +2{1361} + {137} + {14222} +2{1442} + {1451}
+2{146} + {1532} + {1541} + {155} + {1622} +2{164} + {173} + {182} + {20}

{5} ⊗ {4}' = {5555} + {7553} + {7733} + {7751} + {8552} + {8642} + {8741} + {875} + {8822}
+ {9533} +2{9551} + {9632} + {965} +2{9731} + {974} + {983} + {9911} + {10532}
+ {10541} + {1055} + {10631} +2{1064} + {10721} +2{1073} +2{1082} + {1091}
+ {1010} + {11333} +2{11531} + {1154} + {11621} +2{1163} +2{11711} + {1172}
+ {1181} + {12431} + {12521} +2{1253} +2{1262} +2{1271} + {128} + {13331}
+ {1343} +2{13511} + {1352} +2{1361} + {1433} + {14411} + {1442} + {1451}
+ {146} + {15311} + {1541} + {1631} + {17111}

{4} ⊗ {5} = {44444} + {64442} + {66422} + {6644} + {6662} + {74441} + {75431} + {76421}
+ {7643} + {7652} + {7733} + {77411} + {7751} + {84422} +2{8444} + {85421}
+ {8543} + {85511} + {86222} + {86321} +3{8642} + {8651} +2{866} + {87311}
+ {8732} +2{8741} +2{8822} +2{884} + {94421} + {9443} + {95321} + {95411}
+2{9542} + {96221} +2{9632} +3{9641} + {965} + {97211} + {9722} +2{9731} + {974}
+ {9821} + {983} + {104222} +3{10442} + {105221} + {105311} + {10532} +2{10541}
+3{10622} +2{10631} +4{1064} +2{10721} +2{1073} +3{1082} + {1091} + {1010}
+ {114221} + {11432} +2{11441} +2{11522} +2{11531} + {1154} +2{11621} +3{1163}
+ {11711} +2{1172} + {1181} + {122222} +2{12422} + {12431} +3{1244} +2{12521}
+ {1253} +4{1262} + {1271} +2{128} + {13322} + {13421} +2{1343} +2{1352}
+2{1361} + {137} + {14222} +3{1442} + {1451} +2{146} + {1532} + {1541} + {155}
+ {1622} +2{164} + {173} + {182} + {20}

{4} ⊗ {5}' = {5555} + {65531} + {66422} + {75332} + {75521} + {7553} + {76331} + {7643}
+ {7652} + {7733} + {77411} + {7751} + {83333} + {85331} + {85421} + {8543}
+ {85511} + {8552} + {86321} + {8633} +2{8642} + {8651} + {866} + {87311}
+ {8732} +2{8741} + {875} + {8822} + {8831} + {884} + {94331} + {95321} +2{9533}
+ {95411} + {9542} +2{9551} + {96311} +2{9632} +2{9641} + {965} + {97211}
+3{9731} + {974} + {9821} + {983} + {9911} + {103331} + {10433} + {10442}
+2{105311} +2{10532} +2{10541} + {10622} +3{10631} +3{1064} + {107111} +2{10721}
+2{1073} + {10811} +2{1082} + {1010} + {11333} + {114311} + {11432} + {11441}
+ {115211} +3{11531} + {1154} + {116111} +2{11621} +2{1163} +2{11711} + {1172}
+ {1181} + {123311} +2{12431} + {1244} + {125111} +2{12521} + {1253} + {12611}
+2{1262} + {1271} + {13331} + {134111} + {13421} + {1343} +2{13511} + {1361}
+ {143111} + {14411} + {1442} + {15311} + {161111}

{2} ⊗ {10} = {2222222222} + {422222222} + {44222222} + {4442222} + {444422} + {44444}
+ {62222222} + {6422222} + {644222} + {64442} + {662222} + {66422} + {6644}
+ {6662} + {8222222} + {842222} + {84422} + {8444} + {86222} + {8642} + {866}
+ {8822} + {884} + {1022222} + {104222} + {10442} + {10622} + {1064} + {1082}
+ {1010} + {122222} + {12422} + {1244} + {1262} + {128} + {14222} + {1442}
+ {146} + {1622} + {164} + {182} + {20}

The Outer Plethysm of S-Functions of One Part (contd)

{2} ● {10}' = {5555} + {65531} + {66422} + {754211} + {762221} + {8441111} + {8522111}
+ {94211111} + {1031111111} + {11111111111}

{7} ● {3} = {885} + {966} + {1074} + {1083} + {10101} + {1164} + {1182} + {1263} + {1272}
+ {1281} + {129} + {1344} + {1362} + {1371} + {138} + {1452} + {1461} + {147}
+ {1542} +2{156} + {1641} + {165} + {1722} + {174} + {183} + {192} + {21}
{7} ● {3}' = {777} + {975} + {993} + {1074} + {1155} + {1173} + {1182} + {1191} + {1263}
+ {1272} + {129} + {1353} +2{1371} + {138} + {1452} + {1461} + {147} + {1533}
+ {1551} + {156} + {1641} + {165} + {1731} + {183} + {1911}
{3} ● {7} = {55533} + {555411} + {654321} + {65442} + {6552111} + {655311} + {6633111}
+ {664221} + {66441} + {66522} + {6663} + {744222} + {74442} + {7532211}
+ {754221} + {754311} + {75432} + {75441} + {755211} + {75531} + {762222}
+ {763221} + {764211} +2{76422} + {76431} + {7644} + {76521} + {7662} + {772221}
+ {77331} + {77421} + {7743} + {77511} + {8422221} + {844221} + {84432}
+ {84441} + {852222} + {853221} + {853311} + {854211} +2{85422} +2{85431}
+ {8544} + {855111} + {85521} + {862221} + {863211} +2{86322} +3{86421} +2{8643}
+2{8652} + {8661} + {87222} +2{87321} + {87411} +2{8742} + {8751} + {88221}
+ {8832} + {8841} + {885} + {9222222} + {942222} + {943221} +2{94422} + {94431}
+2{9444} + {952221} + {953211} + {95322} + {95331} +3{95421} + {9543} + {95511}
+3{96222} +2{96321} + {9633} + {96411} +4{9642} + {9651} +2{966} + {97221}
+ {97311} +2{9732} +2{9741} +2{9822} + {9831} + {984} + {1032222} + {1042221}
+ {104322} +2{104421} +2{10443} +2{105222} +2{105321} + {105411} +3{10542}
+2{106221} +3{10632} +3{10641} + {1065} +2{10722} +2{10731} +2{1074} + {10821}
+2{1083} + {1092} + {10101} + {1122222} +2{114222} + {114321} +3{11442}
+ {115221} + {115311} +2{11532} +2{11541} +3{11622} +2{11631} +3{1164} +2{11721}
+ {1173} +2{1182} + {123222} + {124221} + {12432} +2{12441} +3{12522} + {12531}
+ {1254} + {12621} +3{1263} +2{1272} + {1281} + {129} + {132222} +2{13422}
+ {13431} +2{1344} + {13521} + {1353} +3{1362} + {1371} + {138} + {14322}
+ {14421} + {1443} +2{1452} + {1461} + {147} + {15222} +2{1542} +2{156} + {1632}
+ {1641} + {165} + {1722} + {174} + {183} + {192} + {21}
{3} ● {7}' = {3333333} + {5333331} + {5533311} + {5553111} + {633333} + {643332}
+ {653331} + {654321} + {655311} +2{66333} + {66432} + {66531} + {6663}
+ {7333311} + {743331} + {74433} + {7533111} + {753321} + {754311} + {75432}
+ {75441} + {7551111} + {755211} + {75522} + {763311} + {76332} + {764211}
+2{76431} + {76521} + {7653} + {76611} + {7731111} + {77322} + {774111}
+ {77421} + {7743} + {7752} + {777} + {833331} + {843321} + {84333} + {84432}
+2{853311} + {85332} + {854211} + {85422} +2{85431} + {8544} + {855111}
+ {85521} + {863211} +3{86331} + {864111} +2{86421} +2{8643} +2{86511} + {8652}
+ {8661} + {873111} +2{87321} + {87411} +2{8742} + {8751} +2{88311} + {8841}
+ {9333111} + {943311} + {94332} +2{94431} + {9444} + {9531111} + {953211}
+ {95322} + {95331} + {954111} +3{95421} + {9543} + {9552} +2{963111} +2{96321}
+2{9633} +3{96411} +2{9642} + {9651} + {9711111} + {972111} + {97221} + {97311}
+2{9732} +2{9741} + {975} + {98211} + {9822} + {9831} + {993} + {1033311}
+ {1043211} + {104331} + {104421} +2{10443} +2{1053111} +2{105321} +2{105411}
+2{10542} + {1062111} + {106221} +3{106311} + {10632} +2{10641} + {1071111}
+ {107211} + {10722} + {10731} + {1074} + {108111} + {10821} + {1133111}
+ {1143111} + {114321} +2{114411} + {11442} + {11511111} + {1152111} + {115221}
+ {115311} + {11532} + {11541} + {1161111} +2{116211} + {11631} + {11721}
+ {1233111} + {1242111} + {124311} + {12441} + {1251111} + {125211} + {12522}
+ {126111} + {13311111} + {1341111} + {134211} + {1431111} + {15111111}

{11} ● {2} = {1210} + {148} + {166} + {184} + {202} + {22}
{11} ● {2}' = {1111} + {139} + {157} + {175} + {193} + {211}
{2} ● {11} = {2222222222} + {4222222222} + {442222222} + {44422222} + {4444222}
+ {444442} + {622222222} + {64222222} + {6442222} + {644422} + {64444}
+ {6622222} + {664222} + {66442} + {66622} + {6664} + {82222222} + {8422222}
+ {844222} + {84442} + {862222} + {86422} + {8644} + {8662} + {88222} + {8842}
+ {886} + {10222222} + {1042222} + {104422} + {10444} + {106222} + {10642}
+ {1066} + {10822} + {1084} + {10102} + {1222222} + {124222} + {12442}
+ {12622} + {1264} + {1282} + {1210} + {142222} + {14422} + {1444} + {1462}
+ {148} + {16222} + {1642} + {166} + {1822} + {184} + {202} + {22}
{2} ● {11}' = {65551} + {66532} + {755311} + {764221} + {772222} + {8542111} + {8622211}
+ {94411111} + {95221111} + {1042111111} + {11311111111} + {121111111111}

The Outer Plethysm of S-Functions

$\{2\} \otimes \{2\} = \{22\} + \{4\}$
$\{2\} \otimes \{11\} = \{31\}$

$\{3\} \otimes \{2\} = \{42\} + \{6\}$
$\{3\} \otimes \{11\} = \{33\} + \{51\}$
$\{21\} \otimes \{2\} = \{222\} + \{3111\} + \{321\} + \{42\}$
$\{21\} \otimes \{11\} = \{2211\} + \{321\} + \{33\} + \{411\}$
$\{2\} \otimes \{3\} = \{222\} + \{42\} + \{6\}$
$\{2\} \otimes \{21\} = \{321\} + \{42\} + \{51\}$
$\{2\} \otimes \{111\} = \{33\} + \{411\}$

$\{4\} \otimes \{2\} = \{44\} + \{62\} + \{8\}$
$\{4\} \otimes \{11\} = \{53\} + \{71\}$
$\{31\} \otimes \{2\} = \{3311\} + \{422\} + \{431\} + \{44\} + \{5111\} + \{521\} + \{62\}$
$\{31\} \otimes \{11\} = \{332\} + \{4211\} + \{431\} + \{521\} + \{53\} + \{611\}$
$\{22\} \otimes \{2\} = \{2222\} + \{3311\} + \{422\} + \{44\}$
$\{22\} \otimes \{11\} = \{3221\} + \{431\}$
$\{2\} \otimes \{4\} = \{2222\} + \{422\} + \{44\} + \{62\} + \{8\}$
$\{2\} \otimes \{31\} = \{3221\} + \{422\} + \{431\} + \{521\} + \{53\} + \{62\} + \{71\}$
$\{2\} \otimes \{22\} = \{3311\} + \{422\} + \{44\} + \{521\} + \{62\}$
$\{2\} \otimes \{211\} = \{332\} + \{4211\} + \{431\} + \{521\} + \{53\} + \{611\}$
$\{2\} \otimes \{1111\} = \{431\} + \{5111\}$

$\{3\} \otimes \{3\} = \{441\} + \{522\} + \{63\} + \{72\} + \{9\}$
$\{3\} \otimes \{21\} = \{432\} + \{531\} + \{54\} + \{621\} + \{63\} + \{72\} + \{81\}$
$\{3\} \otimes \{111\} = \{333\} + \{531\} + \{63\} + \{711\}$
$\{21\} \otimes \{3\} = \{32211\} + \{3222\} + \{33111\} + \{3321\} + \{333\} + \{411111\} + \{42111\} + 2\{4221\}$
$\quad + \{4311\} + \{432\} + \{441\} + \{5211\} + \{522\} + \{531\} + \{63\}$
$\{21\} \otimes \{21\} = \{22221\} + \{321111\} + 2\{32211\} + \{3222\} + \{33111\} + 3\{3321\} + 2\{42111\} + 3\{4221\}$
$\quad + 3\{4311\} + 3\{432\} + \{441\} + \{51111\} + 2\{5211\} + \{522\} + 2\{531\} + \{54\} + \{621\}$
$\{21\} \otimes \{111\} = \{222111\} + \{32211\} + \{3222\} + \{33111\} + \{3321\} + \{333\} + \{42111\} + \{4221\}$
$\quad + 2\{4311\} + \{432\} + \{441\} + \{5211\} + \{522\} + \{531\} + \{6111\}$

$\{5\} \otimes \{2\} = \{64\} + \{82\} + \{10\}$
$\{5\} \otimes \{11\} = \{55\} + \{73\} + \{91\}$
$\{41\} \otimes \{2\} = \{442\} + \{5311\} + \{541\} + \{622\} + \{631\} + \{64\} + \{7111\} + \{721\} + \{82\}$
$\{41\} \otimes \{11\} = \{4411\} + \{532\} + \{541\} + \{55\} + \{6211\} + \{631\} + \{721\} + \{73\} + \{811\}$
$\{32\} \otimes \{2\} = \{3331\} + \{4222\} + \{4321\} + \{442\} + \{5311\} + \{532\} + \{541\} + \{622\} + \{64\}$
$\{32\} \otimes \{11\} = \{3322\} + \{4321\} + \{433\} + \{4411\} + \{5221\} + \{532\} + \{541\} + \{55\} + \{631\}$
$\{311\} \otimes \{2\} = \{33211\} + \{421111\} + \{4222\} + \{43111\} + \{4321\} + \{442\} + \{52111\} + \{5221\}$
$\quad + \{5311\} + \{61111\} + \{622\}$
$\{311\} \otimes \{11\} = \{331111\} + \{3322\} + \{42211\} + \{43111\} + \{4321\} + \{4411\} + \{511111\}$
$\quad + \{52111\} + \{5221\} + \{532\} + \{6211\}$
$\{2\} \otimes \{5\} = \{22222\} + \{4222\} + \{442\} + \{622\} + \{64\} + \{82\} + \{10\}$
$\{2\} \otimes \{41\} = \{32221\} + \{4222\} + \{4321\} + \{442\} + \{5221\} + \{532\} + \{541\} + \{622\} + \{631\}$
$\quad + \{64\} + \{721\} + \{73\} + \{82\} + \{91\}$
$\{2\} \otimes \{32\} = \{33211\} + \{4222\} + \{4321\} + \{442\} + \{5221\} + \{5311\} + \{532\} + \{541\} + 2\{622\}$
$\quad + \{631\} + \{64\} + \{721\} + \{73\} + \{82\}$
$\{2\} \otimes \{311\} = \{3322\} + \{42211\} + \{4321\} + \{433\} + \{4411\} + \{5221\} + \{5311\} + 2\{532\} + \{541\}$
$\quad + \{55\} + \{6211\} + 2\{631\} + \{721\} + \{73\} + \{811\}$
$\{2\} \otimes \{221\} = \{3331\} + \{43111\} + \{4321\} + \{442\} + \{5221\} + \{5311\} + \{532\} + \{541\} + \{6211\}$
$\quad + \{622\} + \{631\} + \{64\} + \{721\}$
$\{2\} \otimes \{2111\} = \{4321\} + \{433\} + \{4411\} + \{52111\} + \{5311\} + \{532\} + \{541\} + \{6211\} + \{631\}$
$\quad + \{7111\}$
$\{2\} \otimes \{11111\} = \{442\} + \{5311\} + \{61111\}$

$\{6\} \otimes \{2\} = \{66\} + \{84\} + \{102\} + \{12\}$
$\{6\} \otimes \{11\} = \{75\} + \{93\} + \{111\}$
$\{51\} \otimes \{2\} = \{5511\} + \{642\} + \{651\} + \{66\} + \{7311\} + \{741\} + \{822\} + \{831\} + \{84\}$
$\quad + \{9111\} + \{921\} + \{102\}$
$\{51\} \otimes \{11\} = \{552\} + \{6411\} + \{651\} + \{732\} + \{741\} + \{75\} + \{8211\} + \{831\} + \{921\}$
$\quad + \{93\} + \{1011\}$
$\{42\} \otimes \{2\} = \{4422\} + \{444\} + \{5331\} + \{5421\} + \{543\} + \{5511\} + \{6222\} + \{6321\} + 2\{642\}$
$\quad + \{651\} + \{66\} + \{7311\} + \{732\} + \{741\} + \{822\} + \{84\}$
$\{42\} \otimes \{11\} = \{4431\} + \{5322\} + \{5421\} + \{543\} + \{552\} + \{6321\} + \{633\} + \{6411\} + \{642\}$
$\quad + \{651\} + \{7221\} + \{732\} + \{741\} + \{75\} + \{831\}$
$\{411\} \otimes \{2\} = \{441111\} + \{4422\} + \{53211\} + \{54111\} + \{5421\} + \{5511\} + \{621111\} + \{6222\}$
$\quad + \{63111\} + \{6321\} + \{642\} + \{72111\} + \{7221\} + \{7311\} + \{81111\} + \{822\}$

The Outer Plethysm of S-functions (contd)

{411} ⊗ {11} = {44211} + {531111} + {5322} + {54111} + {5421} + {552} + {62211} + {63111}
+ {6321} + {6411} + {711111} + {72111} + {7221} + {732} + {8211}

{33} ⊗ {2} = {3333} + {4422} + {5331} + {5511} + {642} + {66}

{33} ⊗ {11} = {4332} + {5421} + {633} + {651}

{321} ⊗ {2} = {332211} + {33321} + {3333} + {42222} + {432111} +2{43221} +2{43311}
+ {4332} + {441111} + {44211} +2{4422} + {4431} + {444} + {522111} + {52221}
+2{53211} + {5322} +2{5331} + {54111} +2{5421} + {543} + {5511} + {6222}
+ {63111} + {6321} + {642}

{321} ⊗ {11} = {33222} + {333111} + {33321} + {422211} + {432111} +2{43221} + {43311}
+2{4332} +2{44211} +2{4431} + {52221} + {531111} +2{53211} +2{5322} + {5331}
+ {54111} +2{5421} + {543} + {552} + {62211} + {6321} + {633} + {6411}

{4} ⊗ {3} = {444} + {642} + {66} + {741} + {822} + {84} + {93} + {102} + {12}

{4} ⊗ {21} = {543} + {642} + {651} + {732} + {741} + {75} + {831} +2{84} + {921} + {93}
+ {102} + {111}

{4} ⊗ {111} = {552} + {633} + {741} + {75} + {831} + {93} + {1011}

{31} ⊗ {3} = {333111} + {43221} + {43311} + {4332} + {44211} +2{4431} + {444} + {531111}
+2{53211} +2{5322} + {5331} + {54111} +4{5421} + {543} +2{552} + {62211}
+ {6222} +2{63111} +3{6321} +2{633} +3{6411} +2{642} + {651} + {711111}
+ {72111} +2{7221} + {7311} +2{732} +2{741} + {75} + {8211} + {822} + {831}
+ {93}

{31} ⊗ {21} = {33321} + {432111} + {43221} +2{43311} +2{4332} +2{44211} +2{4422} +3{4431}
+ {52221} + {531111} +4{53211} +3{5322} +4{5331} +3{54111} +6{5421} +4{543}
+2{5511} +2{552} + {621111} +2{62211} + {6222} +3{63111} +7{6321} +2{633}
+5{6411} +5{642} +3{651} +2{72111} +3{7221} +4{7311} +4{732} +3{741} + {75}
+ {81111} +2{8211} + {822} +2{831} + {84} + {921}

{31} ⊗ {111} = {3333} + {43221} + {43311} + {4332} + {441111} + {44211} + {4422} + {4431}
+ {444} + {522111} +2{53211} + {5322} +3{5331} + {54111} +3{5421} + {543}
+2{5511} + {552} + {62211} + {6222} +2{63111} +3{6321} +2{633} +2{6411}
+3{642} + {651} + {66} + {72111} + {7221} +3{7311} + {732} +2{741} + {8211}
+ {822} + {831} + {9111}

{22} ⊗ {3} = {222222} + {332211} + {3333} + {42222} + {43221} + {43311} + {441111}
+2{4422} + {444} + {53211} + {5331} + {5421} + {5511} + {6222} + {642} + {66}

{22} ⊗ {21} = {322221} + {332211} + {33321} + {42222} + {432111} +2{43221} + {43311}
+ {4332} + {44211} +2{4422} + {4431} + {52221} + {53211} + {5322} + {5331}
+ {54111} +2{5421} + {543} + {5511} + {6321} + {642} + {651}

{22} ⊗ {111} = {33222} + {333111} + {422211} + {43221} + {4332} + {44211} + {4431}
+ {53211} + {5322} + {5421} + {552} + {633} + {6411}

{3} ⊗ {4} = {444} + {5421} + {6222} + {642} + {66} + {732} + {741} + {822} + {84} + {93}
+ {102} + {12}

{3} ⊗ {31} = {4431} + {5322} + {5421} + {543} + {552} + {6321} + {633} + {6411} +2{642}
+ {651} + {7221} +2{732} +2{741} +2{75} + {822} +2{831} + {84} + {921} +2{93}
+ {102} + {111}

{3} ⊗ {22} = {4422} + {5331} + {543} + {5511} + {6321} +2{642} + {651} + {66} + {7311}
+ {732} + {741} + {822} + {831} +2{84} + {921} + {102}

{3} ⊗ {211} = {4332} + {5331} + {5421} + {543} + {552} + {6321} +2{633} + {6411} + {642}
+2{651} + {7311} +2{732} +2{741} + {75} + {8211} +2{831} + {84} + {921} + {93}
+ {1011}

{3} ⊗ {1111} = {3333} + {5331} + {5511} + {633} + {642} + {66} + {7311} + {741} + {831}
+ {9111}

{21} ⊗ {4} =2{332211} +2{33321} + {4221111} + {422211} +2{42222} + {4311111} +3{432111}
+3{43221} +3{43311} +2{4332} + {441111} +2{44211} +3{4422} + {4431} + {444}
+ {51111111} + {5211111} +2{522111} +3{52221} + {531111} +4{53211} +2{5322}
+3{5331} +2{54111} +3{5421} +2{543} + {5511} + {621111} + {62211} +2{6222}
+ {63111} +3{6321} + {6411} +2{642} + {651} + {7311} + {732} + {741} + {84}

{21} ⊗ {31} = {3222111} +2{322221} +2{3321111} +3{332211} +3{33222} +3{333111} +4{33321}
+ {3333} + {42111111} +2{4221111} +5{422211} +2{42222} +2{4311111} +8{432111}
+11{43221} +7{43311} +6{4332} +2{441111} +8{44211} +4{4422} +7{4431}
+2{5211111} +5{522111} +6{52221} +5{531111} +12{53211} +9{5322} +7{5331}
+5{54111} +10{5421} +4{543} +2{5511} +3{552} + {6111111} +2{621111} +5{62211}
+2{6222} +4{63111} +8{6321} +3{633} +5{6411} +4{642} +2{651} + {72111}
+2{7221} +2{7311} +2{732} +2{741} + {75} + {831}

{21} ⊗ {22} = {222222} + {3222111} + {322221} + {33111111} + {3321111} +4{332211}
+ {33222} + {333111} +2{33321} +2{3333} +2{4221111} +2{422211} +3{42222}
+ {4311111} +5{432111} +7{43221} +6{43311} +3{4332} +3{441111} +4{44211}
+6{4422} +3{4431} +2{444} + {5211111} +4{522111} +3{52221} +2{531111}
+9{53211} +4{5322} +6{5331} +3{54111} +7{5421} +2{543} +3{5511} + {552}
+2{621111} +2{62211} +3{6222} +4{63111} +5{6321} + {633} +2{6411} +4{642}
+ {651} + {66} + {72111} + {7221} +2{7311} + {732} + {741} + {822}

{21} ⊗ {211} = {2222211} + {32211111} +2{3222111} +2{322221} +2{3321111} +4{332211}
+3{33222} +3{333111} +4{33321} +2{4221111} +5{422211} +2{42222} +2{4311111}
+8{432111} +10{43221} +7{43311} +7{4332} +2{441111} +9{44211} +4{4422}
+6{4431} + {444} + {5211111} +4{522111} +5{52221} +5{531111} +12{53211}
+8{5322} +7{5331} +6{54111} +11{5421} +4{543} +2{5511} +3{552} +2{621111}
+5{62211} +2{6222} +5{63111} +8{6321} +3{633} +5{6411} +3{642} +2{651}
+ {711111} +2{72111} +2{7221} +2{7311} +2{732} + {741} + {8211}

<u>**The Outer Plethysm of S-functions**</u> (contd)

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{21} ⊗ {1111} = {22221111} + {3222111} + {322221} + {3321111} +2{332211} +2{33321}
              + {3333} + {4221111} + {422211} + {42222} +3{432111} +3{43221} +3{43311}
              + {4332} +2{441111} +2{44211} +3{4422} +2{4431} + {522111} +2{52221}
              + {531111} +4{53211} +2{5322} +3{5331} +3{54111} +3{5421} +2{543} +2{5511}
              + {621111} + {62211} + {6222} +2{63111} +3{6321} + {6411} +2{642} + {72111}
              + {7221} + {7311} + {81111}
{2} ⊗ {6} = {222222} + {42222} + {4422} + {444} + {6222} + {642} + {66} + {822} + {84}
        + {102} + {12}
{2} ⊗ {51} = {322221} + {42222} + {43221} + {4422} + {4431} + {52221} + {5322} + {5421}
           + {543} + {6222} + {6321} +2{642} + {651} + {7221} + {732} + {741} + {75}
           + {822} + {831} + {84} + {921} + {93} + {102} + {111}
{2} ⊗ {42} = {332211} + {42222} + {43221} + {43311} +2{4422} + {444} + {52221} + {53211}
           + {5322} + {5331} +2{5421} + {543} + {5511} +2{6222} +2{6321} +3{642} + {651}
           + {66} + {7221} + {7311} +2{732} +2{741} +2{822} + {831} +2{84} + {921} + {93}
           + {102}
{2} ⊗ {411} = {33222} + {422211} + {43221} + {4332} + {44211} + {4431} + {52221} + {53211}
            +2{5322} + {5331} +2{5421} + {543} +2{552} + {62211} +2{6321} +2{633} +2{6411}
            + {642} + {651} + {7221} + {7311} +2{732} +2{741} + {75} + {8211} +2{831}
            + {921} + {93} + {1011}
{2} ⊗ {33} = {333111} + {43221} + {4431} + {53211} + {5322} + {5421} + {552} + {6222}
           + {6321} + {633} + {6411} + {642} + {7221} + {732} + {741} + {75} + {822}
           + {831} + {93}
{2} ⊗ {321} = {33321} + {432111} + {43221} + {43311} + {4332} + {44211} + {4422} + {4431}
            + {52221} +2{53211} +2{5322} +2{5331} + {54111} +3{5421} +2{543} + {5511}
            + {552} + {62211} + {6222} + {63111} +4{6321} + {633} +2{6411} +3{642} +2{651}
            +2{7221} +2{7311} +3{732} +2{741} + {75} + {8211} + {822} +2{831} + {84}
            + {921}
{2} ⊗ {3111} = {43221} + {4332} + {44211} + {4431} + {522111} + {53211} + {5322} +2{5331}
             + {54111} +2{5421} + {543} + {5511} + {552} + {62211} + {63111} +2{6321}
             +2{633} +2{6411} + {642} + {651} + {72111} +2{7311} + {732} + {741} + {8211}
             + {831} + {9111}
{2} ⊗ {222} = {3333} + {43311} + {441111} + {4422} + {444} + {53211} + {5331} + {5421}
            + {5511} + {6222} + {63111} + {6321} +2{642} + {66} + {7221} + {7311} + {741}
            + {822}
{2} ⊗ {2211} = {43311} + {4332} + {44211} + {4431} + {531111} + {53211} + {5322} + {5331}
             + {54111} +2{5421} + {543} + {552} + {62211} + {63111} +2{6321} + {633}
             +2{6411} + {642} + {651} + {72111} + {7221} + {7311} + {732} + {741} + {8211}
{2} ⊗ {21111} = {4422} + {4431} + {53211} + {5331} + {54111} + {5421} + {543} + {5511}
              + {621111} + {63111} + {6321} + {6411} + {642} + {72111} + {7311} + {81111}
{2} ⊗ {111111} = {444} + {5421} + {63111} + {711111}


{7} ⊗ {2} = {86} + {104} + {122} + {14}
{7} ⊗ {11} = {7.} + {95} + {113} + {131}
{61} ⊗ {2} = {662} + {7511} + {761} + {842} + {851} + {86} + {9311} + {941} + {1022}
           + {1031} + {104} + {11111} + {1121} + {122}
{61} ⊗ {11} = {6611} + {752} + {761} + {77} + {8411} + {851} + {932} + {941} + {95}
            + {10211} + {1 31} + {1121} + {113} + {1211}
{52} ⊗ {2} = {5531} + {6422} + {644} + {6521} + {653} + {662} + {7331} + {7421} + {743}
           + {7511} + {752} + {761} + {8222} + {8321} +2{842} + {851} + {86} + {9311}
           + {932} + {941} + {1022} + {104}
{52} ⊗ {11} = {5522} + {554} + {6431} + {6521} + {653} + {6611} + {7322} + {7421} + {743}
            +2{752} + {761} + {77} + {8321} + {833} + {8411} + {842} + {851} + {9221}
            + {932} + {941} + {95} + {1031}
{511} ⊗ {2} = {55211} + {641 11} + {6422} + {65111} + {6521} + {662} + {73211} + {74111}
            + {7421} + {7511} + {821111} + {8222} + {83111} + {8321} + {842} + {92111}
            + {9221} + {9311} + {101111} + {1022}
{511} ⊗ {11} = {551111} + {5522} + {64211} + {65111} + {6521} + {6611} + {731111} + {7322}
             + {74111} + {7421} + {752} + {82211} + {83111} + {8321} + {8411} + {911111}
             + {92111} + {9221} + {932} + {10211}
{43} ⊗ {2} = {4442} + {5333} + {5432} + {5531} + {6422} + {6431} + {644} + {6521} + {662}
           + {7331} + {743} + {7511} + {752} + {761} + {842} + {86}
{43} ⊗ {11} = {4433} + {5432} + {5441} + {5522} + {6332} + {6431} + {6521} + {653}
            + {6611} + {7421} + {743} + {752} + {761} + {77} + {833} + {851}
{421} ⊗ {2} = {44222} + {443111} + {44321} + {4442} + {532211} + {53321} + {5333}
            + {542111} +2{54221} +2{54311} +2{5432} + {5441} +2{55211} +2{5531} + {62222}
            + {632111} +2{63221} +2{63311} + {6332} + {641111} +2{64211} +3{6422} +2{6431}
            + {644} + {65111} +2{6521} + {653} + {662} + {722111} + {72221} +2{73211}
            + {7322} +2{7331} + {74111} +2{7421} + {743} + {7511} + {8222} + {83111}
            + {8321} + {842}
```

The Outer Plethysm of S-Functions (contd)

{421} ⊗ {11} = {442211} + {44321} + {4433} + {44411} + {53222} + {533111} + {53321}
+ {542111} +2{54221} +2{54311} +2{5432} + {5441} + {551111} + {55211}
+2{5522} + {5531} + {554} + {622211} + {632111} +2{63221} + {63311} +2{6332}
+3{64211} + {6422} +3{6431} + {65111} +2{6521} + {653} + {6611} + {72221}
+ {731111} +2{73211} +2{7322} + {7331} + {74111} +2{7421} + {743} + {752}
+ {82211} + {8321} + {833} + {8411}

{4111} ⊗ {2} = {4421111} + {44222} + {53111111} + {532211} + {5411111} + {542111}
+ {54221} + {55211} + {6221111} + {62222} + {6311111} + {632111} + {63221}
+ {641111} + {6422} + {71111111} + {7211111} + {722111} + {72221} + {73211}
+ {821111} + {8222}

{4111} ⊗ {11} = {44111111} + {442211} + {5321111} + {53222} + {5411111} + {542111}
+ {54221} + {551111} + {5522} + {62111111} + {622211} + {6311111} + {632111}
+ {63221} + {64211} + {7211111} + {722111} + {72221} + {731111} + {7322}
+ {8111111} + {82211}

{331} ⊗ {2} = {33332} + {433211} + {43331} + {44222} + {44321} + {4442} + {53321} + {5333}
+ {542111} + {54221} + {54311} + {5432} + {55211} + {5531} + {63311} + {6422}
+ {6431} + {644} + {65111} + {6521} + {662}

{331} ⊗ {11} = {333311} + {43322} + {43331} + {442211} + {44321} + {4433} + {533111}
+ {53321} + {54221} + {54311} + {5432} + {5441} + {551111} + {55211} + {5522}
+ {6332} + {64211} + {6431} + {6521} + {653} + {6611}

{2} ⊗ {7} = {2222222} + {422222} + {44222} + {4442} + {62222} + {6422} + {644} + {662}
+ {8222} + {842} + {86} + {1022} + {104} + {122} + {14}

{2} ⊗ {61} = {3222221} + {422222} + {432221} + {44222} + {44321} + {4442} + {522221}
+ {53222} + {54221} + {5432} + {5441} + {62222} + {63221} +2{6422} + {6431}
+ {644} + {6521} + {653} + {662} + {72221} + {7322} + {7421} + {743} + {752}
+ {761} + {8222} + {8321} +2{842} + {851} + {86} + {9221} + {932} + {941}
+ {95} + {1022} + {1031} + {104} + {1121} + {113} + {122} + {131}

{2} ⊗ {52} = {3322211} + {422222} + {432221} + {433211} +2{44222} + {44321} + {4442}
+ {522221} + {532211} + {53222} + {53321} +2{54221} + {54311} +2{5432} + {5441}
+ {55211} + {5531} +2{62222} +2{63221} + {63311} +4{6422} +2{6431} +2{644}
+2{6521} + {653} +2{662} + {72221} + {73211} +2{7322} + {7331} +3{7421} +2{743}
+ {7511} +2{752} + {761} +2{8222} +2{8321} +4{842} +2{851} + {86} + {9221}
+ {9311} +2{932} +2{941} + {95} +2{1022} + {1031} +2{104} + {1121} + {113}
+ {122}

{2} ⊗ {511} = {332222} + {4222211} + {432221} + {43322} + {442211} + {44321} + {4433}
+ {44411} + {522221} + {532211} +2{53222} + {53321} +2{54221} + {54311}
+2{5432} + {5441} +2{5522} + {5531} + {554} + {622211} +2{63221} +2{6332}
+2{64211} + {6422} +3{6431} +2{6521} +2{653} + {6611} + {72221} + {73211}
+2{7322} + {7331} +3{7421} +2{743} + {7511} +3{752} + {761} + {77} + {82211}
+2{8321} +2{833} +2{8411} + {842} +2{851} + {9221} + {9311} +2{932} +2{941}
+ {95} + {10211} +2{1031} + {1121} + {113} + {1211}

{2} ⊗ {43} = {3332111} + {432221} + {433211} + {44222} + {44321} + {4442} + {532211}
+ {53222} + {533111} + {53321} +2{54221} + {54311} + {5432} + {5441} + {55211}
+ {5522} + {5531} + {62222} +2{63221} + {63311} + {6332} + {64211} +3{6422}
+2{6431} + {644} +2{6521} + {653} + {662} + {72221} + {73211} +2{7322} + {7331}
+3{7421} +2{743} + {7511} +2{752} + {761} +2{8222} +2{8321} + {833} + {8411}
+3{842} + {851} + {86} + {9221} +2{932} +2{941} + {95} + {1022} + {1031}
+ {104} + {113}

{2} ⊗ {421} = {333221} + {4322111} + {432221} + {433211} + {43322} + {43331} + {442211}
+ {44222} + {443111} +2{44321} + {4442} + {522221} +2{532211} +2{53222}
+ {533111} +3{53321} + {5333} + {542111} +4{54221} +3{54311} +4{5432} +2{5441}
+2{55211} +2{5522} +3{5531} + {554} + {622211} + {62222} + {632111} +4{63221}
+3{63311} +3{6332} +4{64211} +5{6422} +5{6431} +2{644} + {65111} +5{6521}
+3{653} + {6611} +2{662} +2{72221} +3{73211} +4{7322} +4{7331} + {74111}
+7{7421} +4{743} +3{7511} +4{752} +2{761} + {82211} + {8222} + {83111}
+5{8321} +2{833} +3{8411} +5{842} +3{851} + {86} +2{9221} +2{9311} +3{932}
+3{941} + {95} + {10211} + {1022} +2{1031} + {104} + {1121}

{2} ⊗ {4111} = {432221} + {43322} + {442211} + {44321} + {4433} + {44411} + {5222111}
+ {532211} + {53222} +2{53321} + {5333} + {542111} +2{54221} +2{54311}
+2{5432} + {5441} + {55211} +2{5522} +2{5531} + {554} + {622211} + {632111}
+2{63221} + {63311} +3{6332} +3{64211} + {6422} +4{6431} + {65111} +3{6521}
+2{653} + {6611} + {722111} +2{73211} + {7322} +3{7331} +2{74111} +3{7421}
+2{743} +2{7511} +2{752} + {761} + {82211} + {83111} +2{8321} +2{833}
+3{8411} + {842} + {851} + {92111} +2{9311} + {932} + {941} + {10211}
+ {1031} + {11111}

{2} ⊗ {331} = {333311} + {4331111} + {433211} + {43322} + {442211} + {44321} + {4433}
+ {44411} + {532211} + {53222} + {533111} +2{53321} + {542111} +2{54221}
+2{54311} +2{5432} + {5441} + {55211} +2{5522} + {5531} + {554} + {632111}
+3{63221} + {63311} +2{6332} +3{64211} +2{6422} +4{6431} + {65111} +3{6521}
+2{653} + {6611} + {72221} +2{73211} +3{7322} +2{7331} + {74111} +4{7421}
+2{743} + {7511} +3{752} + {761} + {77} + {82211} + {8222} +3{8321} +2{833}
+2{8411} +2{842} +2{851} + {9221} + {9311} +2{932} + {941} + {95} + {1031}

The Outer Plethysm of S-functions (contd)

{2} • {322} = {33332} + {433211} + {43331} + {4421111} + {44222} + {443111} + {44321}
+ {4442} + {532211} + {533111} +2{53321} + {5333} + {542111} +2{54221}
+2{54311} +2{5432} + {5441} +2{55211} +2{5531} + {62222} + {632111} +2{63221}
+3{63311} + {6332} + {641111} +2{64211} +4{6422} +3{6431} +2{644} + {65111}
+3{6521} + {653} +2{662} + {72221} +3{73211} +2{7322} +2{7331} + {74111}
+4{7421} +2{743} +2{7511} +2{752} + {761} +2{8222} + {83111} +3{8321} + {8411}
+3{842} + {851} + {86} + {9221} + {9311} + {932} + {941} + {1022}

{2} • {3211} = {433211} + {43322} + {43331} + {442211} + {443111} +2{44321} + {4433}
+ {44411} + {5321111} + {532211} + {53222} + {533111} +3{53321} + {5333}
+2{542111} +3{54221} +4{54311} +4{5432} +2{5441} + {551111} +2{55211}
+2{5522} +3{5531} + {554} + {622211} +2{632111} +3{63221} +3{63311} +4{6332}
+ {641111} +6{64211} +3{6422} +6{6431} + {644} +2{65111} +5{6521} +3{653}
+2{6611} + {662} + {722111} + {72221} + {731111} +4{73211} +3{7322} +4{7331}
+3{74111} +6{7421} +3{743} +3{7511} +3{752} + {761} +2{82211} +2{83111}
+4{8321} +2{833} +3{8411} +2{842} +2{851} + {92111} + {9221} +2{9311} + {932}
+ {941} + {10211}

{2} • {31111} = {44222} + {44321} + {4442} + {532211} + {53321} + {5333} + {542111}
+ {54221} +2{54311} +2{5432} + {5441} +2{55211} +2{5531} + {6221111}
+ {632111} + {63221} +2{63311} + {6332} + {641111} +2{64211} +2{6422}
+3{6431} + {644} +2{65111} +2{6521} + {653} + {662} + {722111} + {731111}
+2{73211} +2{7331} +2{74111} +2{7421} + {743} +2{7511} + {821111} +2{83111}
+ {8321} + {8411} + {842} + {92111} + {9311} + {101111}

{2} • {2221} = {43331} + {443111} + {44321} + {4442} + {533111} + {53321} + {5333}
+ {5411111} + {542111} + {54221} +2{54311} + {5432} + {5441} + {55211}
+ {5522} + {5531} + {632111} + {63221} +2{63311} + {6332} + {641111}
+2{64211} +2{6422} +2{6431} + {644} + {65111} +2{6521} + {653} + {662}
+ {72221} + {731111} +2{73211} + {7322} + {7331} + {74111} +3{7421} + {743}
+ {7511} + {752} + {761} + {82211} + {8222} + {83111} + {8321} + {8411}
+ {842} + {9221}

{2} • {22111} = {44321} + {4433} + {44411} + {533111} + {53321} + {542111} + {54221}
+2{54311} +2{5432} + {5441} + {551111} + {55211} + {5522} + {5531} + {554}
+ {6311111} + {632111} + {63221} + {63311} + {6332} + {641111} +3{64211}
+ {6422} +3{6431} + {65111} +2{6521} + {653} + {6611} + {722111} + {731111}
+2{73211} + {7322} + {7331} +2{74111} +2{7421} + {743} + {7511} + {752}
+ {821111} + {82211} + {83111} + {8321} + {8411} + {92111}

{2} • {211111} = {4442} + {54221} + {54311} + {5432} + {5441} + {55211} + {5531}
+ {632111} + {63311} + {641111} + {64211} + {6422} + {6431} + {644}
+ {65111} + {6521} + {7211111} + {731111} + {73211} + {74111} + {7421}
+ {821111} + {83111} + {911111}

{2} • {1111111} = {5441} + {5522} + {64211} + {731111} + {8111111}

APPENDIX IV

PUBLICATIONS

A large part of the results of this thesis have been, or are being, published, in co-authorship with B.G. Wybourne. Most of Chapters I to III, with the exception of the section on the calculation of plethysms have been published:

"The Configurations $(d+s)^N$ and the Group R_6", J. Phys. 30, 181 (1969).

"Applications of S-Functional Analysis to Continuous Groups in Physics", J. Phys. 30, 795 (1969).

"Reduction of the Kronecker Products for Rotation Groups", J. Phys. 30, 655 (1969).

The results of Chapter V have not been published. Chapters IV and VI are in press with J. Math. Phys. under the titles:

"Generalized Racah Tensors and the Structure of Mixed Configurations".

"Is the Group R_4 an Approximate Symmetry for Many Electron Theory?"

Some of these results are to be published also in the Proceedings of the NATO Advanced Study Institute, Izmir, Turkey, 1969.

Many of the tables produced by the computer programmes are included as an appendix of 200 pages to the book, B.G. Wybourne, "Symmetry Principles and Atomic Spectroscopy", (John Wiley and Sons, New York, 1970) (in press).